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# **pyspeckit Documentation**

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An [extensible](#) spectroscopic analysis toolkit for astronomy.

If you're just getting started, see the [examples page](#).

To cite pyspeckit, use <http://adsabs.harvard.edu/abs/2011ascl.soft09001G>.



# **Part I**

## **Downloads**





- April 2017 version
- latest commit from [github](#) (same as above, or also *Install pyspeckit via GitHub*)
- latest commit from [bitbucket](#) (see *Installation and Requirements*)
- [pypi](#) entry.

Supported file types and their formats:

- *FITS*
- *Plain Text*
- *hdf5*



## **Part II**

# **Guides / Getting Started**



If you're already a python user, go straight to the [examples page](#) to get a quick start. For simple gaussian fitting, [this example](#) is a good starting point.

- ***Guide for GILDAS-CLASS users***

A simple getting started guide aimed at Gildas-CLASS users

- ***Guide for IRAF users***

Intended for users of IRAF's splot interactive fitting routine.



## **Part III**

# **Classes and API**





At the core, PySpecKit runs on a ‘Spectroscopic Object’ class called [Spectrum](#). Therefore everything interesting about PySpecKit can be learned by digging into the properties of this class.

- [spectrum](#) can read a variety of individual spectra types
  - [Spectrum](#) The Spectrum class, which is the core of pyspeckit. The `__init__` procedure opens a spectrum file.
  - [Spectra](#) A group of [Spectrum](#) s. Generally for when you have multiple wavelength observations you want to stitch together (e.g., two filterbanks on a heterodyne system, or the red/blue spectra from a multi-band spectrometer like the Double Imaging Spectrograph)
  - [ObsBlock](#) An Observation Block - multiple spectra of different objects or different times covering the same wavelength range
- [Cubes](#) is used to deal with data cubes and has functionality similar to [GAIA](#) and [ds9](#).
  - [Cube](#) A Cube of Spectra. Has features to collapse the cube along the spectral axis and fit spectra to each element of the cube. Is meant to replicate [Starlink’s GAIA](#) in some ways, but with less emphasis on speed and much greater emphasis on spectral line fitting.



# **Part IV**

## **Features**



- *Baseline Fitting* describes baseline & continuum fitting.
- *Model Fitting* describes the general process of model fitting.
- *Measurements* is a toolkit for performing EQW, column, and other measurements. . .
- *Units* contains the all-important `SpectroscopicAxis` class that is used to deal with coordinate transformations
- *Registration* describes the extensible qualities of pyspeckit



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## Installation and Requirements

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**Hint:** You can *pip install* pyspeckit to get the latest release version:

```
pip install pyspeckit
```

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PySpecKit requires at least the basic scientific packages:

- [numpy](#)
- [matplotlib](#)
- [mpfit](#) is included
- [scipy](#) is optional. It is only required for RADEX grid interpolation and certain types of optimization
- [python2.7](#) or [ordereddict](#) for model parameter storage

You'll most likely want at least one of the following packages to enable [file reading](#)

- [astropy](#) >=0.4
- [pyfits](#) >=2.4
- [atpy](#) (which depends on [asciitable](#) [[github link](#)] )
- [hdf5](#)

If you have pip (see <http://pypi.python.org/pypi/pyspeckit>), you can install with:

```
pip install pyspeckit
```

Or the most recent version with either of these commands:

```
pip install https://github.com/pyspeckit/pyspeckit/archive/master.zip  
pip install https://bitbucket.org/pyspeckit/pyspeckit/get/master.tar.gz
```

You can acquire the code with this clone command (see also *Install pyspeckit via GitHub*):

```
git clone git@bitbucket.org:pyspeckit/pyspeckit.git pyspeckit
cd pyspeckit
python setup.py install
```

Or you can [Download the latest tarball version](#), then extract and install using the standard python method (but the pip install version of this is easier):

```
wget --no-check-certificate https://bitbucket.org/pyspeckit/pyspeckit/get/master.tar.gz
tar -xzf master.tar.gz
cd pyspeckit-pyspeckit-[commit]
python setup.py install
```

You can also check out the [source code](#)

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**Note:** If you use `easy_install pyspeckit` with the Enthought Python Distribution, you will most likely get a `SandboxViolation` error. You can get around this by using `python setup.py install` or `pip install pyspeckit`.

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**Note:** `pyspeckit` is hosted on both `bitbucket` and `github`. Both versions are kept up to date, so it should not matter which one you choose to install.

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## 1.1 Install pyspeckit via GitHub

### 1.1.1 Quick

You can pip install the development version of `pyspeckit`:

```
pip install https://github.com/pyspeckit/pyspeckit/archive/master.zip
```

### 1.1.2 Installing a branch

If there's a bugfix branch, e.g., from a pull request, you can install it in a similar way. Just replace the branch name:

```
pip install https://github.com/pyspeckit/pyspeckit/archive/{branchname}.zip
```

Or, if the contribution is from a different user:

```
pip install https://github.com/{username}/pyspeckit/archive/{branchname}.zip
```

Where in both cases you need to replace `{{branchname}}` and `{username}`.

### 1.1.3 More detailed

If you want to help develop `pyspeckit`, follow these instructions:

Logged into your github account, go to <https://github.com/pyspeckit/pyspeckit> and click “Fork” in upper right.

Copy the URL of your `pyspeckit` fork <https://github.com/yourusername/pyspeckit>



On the command line type:

```
git clone https://github.com/yourusername/pyspeckit
```

(it will put it in a directory called pyspeckit in your working directory):

```
cd pyspeckit  
git remote add upstream https://github.com/pyspeckit/pyspeckit
```

To get the most up to date version, type:

```
git pull upstream master
```

Update your personal “fork” to match upstream/master:

```
git push origin master
```

and enter your username and password if it asks.

Still in the pyspeckit/ directory, type:

```
python setup.py develop
```

You’re good to go!

### 1.1.4 To make changes and generate a Pull request:

Create a new branch: `git checkout -b name_of_your_new_branch` This will automatically switch you to this new branch. Type `git branch` to see all the branches. The active one will be highlighted and have an asterisk next to it. To switch to an existing branch, type `git checkout name_of_branch`

After you make a change inside your local fork on your machine, type `git add changed_file` where `changed_file` is the name of the file(s) you edited.

Time to commit your change and add a little note about your change `git commit -m details` details should be a description of the changes you made, inside quotes

Push the change to GitHub: `git push origin name_of_branch` where `name_of_branch` is the branch you’ve been active in during this process.

If you want to contribute your changes to <https://github.com/pyspeckit/pyspeckit>, create a “pull request”. In <https://github.com/yourusername/pyspeckit>, navigate to your branch where you pushed you want to merge with <https://github.com/pyspeckit/pyspeckit> and click “Pull request”



See [Parameters](#) for information on how to restrict/modify model parameters.

The generic `SpectralModel` class is a wrapper for model functions. A model should take in an X-axis and some number of parameters. In order to declare a `SpectralModel`, you give `SpectralModel` the function name and the number of parameters it requires. The rest of the options are optional, though `parnames` & `shortvarnames` are strongly recommended. If you do not specify `fitunits`, your fitting code must deal with units internally.

Here are some examples of how to make your own fitters:

```
hill5_fitter = model.SpectralModel(hill5_model, 5,
    parnames=['tau', 'v_lsr', 'v_infall', 'sigma', 'tpeak'],
    parlimited=[(True,False),(False,False),(True,False),(True,False), (True,False)],
    parlimits=[(0,0), (0,0), (0,0), (0,0), (0,0)],
    # specify the parameter names (TeX is OK)
    shortvarnames=("\\tau", "v_{lsr}", "v_{infall}", "\\sigma", "T_{peak}"),
    fitunits='Hz' )

gaussfitter = model.SpectralModel(gaussian, 3,
    parnames=['amplitude', 'shift', 'width'],
    parlimited=[(False,False),(False,False),(True,False)],
    parlimits=[(0,0), (0,0), (0,0)],
    shortvarnames=('A', r'\Delta x', r'\sigma'))
```

Then you can [register](#) these fitters.



Once you have a model defined, you can fit it using the `pyspeckit.Spectrum.specfit` module. Documents on fitting have not been prepared yet, but you can learn most of the tricks by looking at the various fitting examples and the [Parameters](#) documentation.

## 3.1 Related Documents

### 3.1.1 Parameters

Model parameters are very flexible, and can be accessed and modified in many parallel ways.

The `parinfo` class is built on top of `lmfit-py`'s [parameters](#) for compatibility with `lmfit-py`, but it builds on that. The code for the parameter overloading is in `parinfo.py`.

#### Simple Example

Start with a simple example: if you want to limit parameters to be within some range, use the `limits` and `limited` parameters.

```
# define shorthand first:
T,F = True,False
sp.specfit(fittype='gaussian', guesses=[-1,5,1,0.5,2,1],
           limits=[(0,0), (0,0), (0,0), (0,0), (0,0), (0,0)],
           limited=[(F,T), (F,F), (T,F), (T,F), (F,F), (T,F)])
```

In this example, there are two gaussian components being fitted because a Gaussian takes 3 parameters, an amplitude, a center, and a width, and there are 6 parameters in the input guesses.

The first line is forced to be an absorption line: its limits are  $(0,0)$  but `limited=(F,T)` so only the 2nd parameter, the upper limit, is respected: the amplitude is forced to be  $A \leq 0$ .

The second line has its amplitude (the 4th parameter in guesses) forced *positive* since its limits are also  $(0,0)$  but its `limited=(T,F)`.

Both lines have their *widths* forced to be positive, which is true by default: there is no meaning to a negative width, since the width enters into the equation for a gaussian as  $\sigma^2$ .

Note that the need to limit parameters is the main reason for the existence of `lmfit-py` and `mpfit`.

## Tying Parameters

It is also possible to explicitly state that one parameter depends on another. If, for example, you want to fit two gaussians, but they must be at a fixed wavelength separation from one another (e.g., for fitting the [S II] doublet), use `tied`:

```
sp.specfit(fittype='gaussian', guesses=[1,6716,1,0.5,6731,1],
          tied=['', '', '', '', 'p[1]', ''])
```

If you use `lmfit-py` by specifying `use_lmfit=True`, you can use the more advanced [mathematical constraints](#) permitted by `lmfit-py`.

*Optical fitting: The H $\alpha$ -[NII] complex of a type-I Seyfert galaxy* shows a more complete example using `tied`.

## Making your own parinfo

You can also build a `parinfo` class directly. Currently, the best example of this is in `tests/test_formaldehyde_mm_radex.py`.

Here's an example of how you would set up a fit using `parinfo` directly.

**Warning:** There is a bug in the `use_lmfit` section of this code that keeps it from working properly. =(

```
amplitude0 = pyspeckit.parinfo.Parinfo(n=0, parname='Amplitude0',
    shortparname='$A_0$', value=1, limits=[0, 100], limited=(True,True))
width0 = pyspeckit.parinfo.Parinfo(n=2, parname='Width0',
    shortparname='$\sigma_0$', value=1, limits=(0, 0), limited=(True,False))
center0 = pyspeckit.parinfo.Parinfo(n=1, parname='Center0',
    shortparname='$\Delta x_0$', value=6716, limits=(0, 0), limited=(False,False))
amplitude1 = pyspeckit.parinfo.Parinfo(n=3, parname='Amplitude1',
    shortparname='$A_1$', value=1, limits=[0, 100], limited=(True,True))
width1 = pyspeckit.parinfo.Parinfo(n=5, parname='Width1',
    shortparname='$\sigma_1$', value=1, limits=(0, 0), limited=(True,False))
center1 = pyspeckit.parinfo.Parinfo(n=4, parname='Center1',
    shortparname='$\Delta x_1$', value=6731, limits=(0, 0),
    limited=(False,False), tied=center0)

parinfo = pyspeckit.parinfo.ParinfoList([amplitude0,center0,width0,amplitude1,center1,width1])

sp.specfit(parinfo=parinfo, use_lmfit=True)
```

## 3.2 Generic Models and Tools

### 3.2.1 Gaussian Model

The Gaussian model implements a Gaussian function and wraps it in the generic fitter tools.

The simplest and most useful model.

Until 12/23/2011, gaussian fitting used the complicated and somewhat bloated gaussfitter.py code. Now, this is a great example of how to make your own model! Just make a function like gaussian and plug it into the SpectralModel class.

## Module API

```
pyspeckit.spectrum.models.inherited_gaussfitter.gaussian(xarr,    amplitude,    dx,    width,
                                                         return_components=False,
                                                         normalized=False,                re-
                                                         turn_hyperfine_components=False)
```

Returns a 1-dimensional gaussian of form  $A \cdot \exp(-(x-dx)^2/(2 \cdot w^2))$

Area is  $\sqrt{2 \cdot \pi \cdot \sigma^2} \cdot \text{amplitude}$  - i.e., this is NOT a normalized gaussian, unless `normalized=True` in which case  $A = \text{Area}$

### Parameters

#### **xarr**

[np.ndarray] array of x values

#### **amplitude**

[float] Amplitude of the Gaussian, i.e. its peak value, unless `normalized=True` then A is the area of the gaussian

#### **dx**

[float] Center or “shift” of the gaussian

#### **width**

[float] Width of the gaussian (sigma)

#### **return\_components**

[bool] dummy variable; `return_components` does nothing but is required by all fitters

#### **return\_hyperfine\_components**

[bool] dummy variable; does nothing but is required by all fitters

#### **normalized**

[bool] Return a normalized Gaussian?

```
pyspeckit.spectrum.models.inherited_gaussfitter.gaussian_fitter()
```

Generator for Gaussian fitter class

```
pyspeckit.spectrum.models.inherited_gaussfitter.gaussian_integral(amplitude, sigma)
```

Integral of a Gaussian

```
pyspeckit.spectrum.models.inherited_gaussfitter.gaussian_vheight_fitter()
```

Generator for Gaussian fitter class

## 3.2.2 Voigt Profile model

### Module API

```
pyspeckit.spectrum.models.inherited_voigtfitter.voigt(xarr, amp, xcen, sigma, gamma, normal-
                                                         ized=False)
```

Normalized Voigt profile

$$z = (x+i \cdot \text{gam})/(\text{sig} \cdot \sqrt{2}) \quad V(x, \text{sig}, \text{gam}) = \text{Re}(w(z))/(\text{sig} \cdot \sqrt{2 \cdot \pi})$$

The area of  $V$  in this definition is 1. If `normalized=False`, then you can divide the integral of  $V$  by  $\sigma\sqrt{2\pi}$  to get the area.

Original implementation converted from <http://mail.scipy.org/pipermail/scipy-user/2011-January/028327.html> (had an incorrect normalization and strange treatment of the input parameters)

Modified implementation taken from wikipedia, using the definition. [http://en.wikipedia.org/wiki/Voigt\\_profile](http://en.wikipedia.org/wiki/Voigt_profile)

#### Parameters

**xarr**

[np.ndarray] The X values over which to compute the Voigt profile

**amp**

[float] Amplitude of the voigt profile if `normalized = True`, `amp` is the AREA

**xcen**

[float] The X-offset of the profile

**sigma**

[float] The width / sigma parameter of the Gaussian distribution

**gamma**

[float] The width / shape parameter of the Lorentzian distribution

**normalized**

[bool] Determines whether “`amp`” refers to the area or the peak of the voigt profile

`pyspeckit.spectrum.models.inherited_voigtfitter.voigt_fitter()`

Generator for voigt fitter class

`pyspeckit.spectrum.models.inherited_voigtfitter.voigt_fwhm(sigma, gamma)`

Approximation to the Voigt FWHM from wikipedia

[http://en.wikipedia.org/wiki/Voigt\\_profile](http://en.wikipedia.org/wiki/Voigt_profile)

#### Parameters

**sigma**

[float] The width / sigma parameter of the Gaussian distribution

**gamma**

[float] The width / shape parameter of the Lorentzian distribution

`pyspeckit.spectrum.models.inherited_voigtfitter.voigt_moments(self, *args, **kwargs)`

Get the spectral moments from the moments package. Use the gaussian width for the lorentzian width (not a great guess!)

### 3.2.3 LTE Molecule Model

There is a tool for modeling the full LTE spectrum of a molecule. It uses the CDMS / VAMDC database ([http://portal.vamdc.eu/vamdc\\_portal/home.seam](http://portal.vamdc.eu/vamdc_portal/home.seam)) and the `vamdcclib` (<http://vamdcclib.readthedocs.io>) python library to compute the partition function of a molecule. It uses `astroquery.splatalogue` (<http://astroquery.readthedocs.io/en/latest/splatalogue/splatalogue.html>) to identify the line frequencies and energy levels.

A very simple example looks like this:



```
freqs, aij, deg, EU, partfunc = get_molecular_parameters('CH3OH',
                                                         fmin=90*u.GHz,
                                                         fmax=100*u.GHz)

def modfunc(xarr, vcen, width, tex, column):
    return generate_model(xarr, vcen, width, tex, column, freqs=freqs, aij=aij,
                        deg=deg, EU=EU, partfunc=partfunc)

fitter = generate_fitter(modfunc, name="CH3OH")
```

The molecular parameter lookup stage is often slow and may be a bottleneck.

Details can be found in the API documentation:

## LTE Molecule Modeling Tool

Uses astroquery & vamdclib to obtain molecular parameters. <http://astroquery.readthedocs.io/en/latest/splatalogue/splatalogue.html>

Equations are based on Mangum & Shirley 2015 (2015PASP..127..266M)

## Module API

`pyspeckit.spectrum.models.lte_molecule.Jnu(nu, T)`

RJ equivalent temperature (MS15 eqn 24)

`pyspeckit.spectrum.models.lte_molecule.Jnu_cgs(nu, T)`

RJ equivalent temperature (MS15 eqn 24) (use cgs constants for speed)

`pyspeckit.spectrum.models.lte_molecule.generate_fitter(model_func, name)`

Generator for hnco fitter class

`pyspeckit.spectrum.models.lte_molecule.generate_model(xarr, vcen, width, tex, column, freqs,  
aij, deg, EU, partfunc, background=None,  
tbg=2.73)`

Model Generator

`pyspeckit.spectrum.models.lte_molecule.get_molecular_parameters(molecule_name,  
molecule_name_vamdc=None,  
tex=50, fmin=<Quantity 1.0 GHz>, fmax=<Quantity 1.0 THz>,  
line_lists=['SLAIM'],  
chem_re_flags=0, **kwargs)`

Get the molecular parameters for a molecule from the CDMS database using vamdclib

### Parameters

#### **molecule\_name**

[string] The string name of the molecule (normal name, like CH3OH or CH3CH2OH)

#### **molecule\_name\_vamdc**

[string or None] If specified, gives this name to vamdc instead of the normal name. Needed for some molecules, like CH3CH2OH -> C2H5OH.

#### **tex**

[float] Optional excitation temperature (basically checks if the partition function calculator works)

**fmin**

[quantity with frequency units]

**fmax**

[quantity with frequency units] The minimum and maximum frequency to search over

**line\_lists**

[list] A list of Splatalogue line list catalogs to search. Valid options include SLAIM, CDMS, JPL. Only a single catalog should be used to avoid repetition of transitions and species

**chem\_re\_flags**

[int] An integer flag to be passed to splatalogue's chemical name matching tool

## Examples

```

>>> freqs, aij, deg, EU, partfunc = get_molecular_parameters(molecule_name='CH2CHCN',
...                                                         fmin=220*u.GHz,
...                                                         fmax=222*u.GHz,
...                                                         molecule_name_vamdc='C2H3CN')
>>> freqs, aij, deg, EU, partfunc = get_molecular_parameters('CH3OH',
...                                                         fmin=90*u.GHz,
...                                                         fmax=100*u.GHz)

```

pyspeckit.spectrum.models.lte\_molecule.**line\_tau**(*tex*, *total\_column*, *partition\_function*, *degeneracy*, *frequency*, *energy\_upper*, *einstein\_A*=None)

Given the excitation temperature of the state, total column density of the molecule, the partition function, the degeneracy of the state, the frequency of the state, and the upper-state energy level, return the optical depth of that transition.

This is a helper function for the LTE molecule calculations. It implements the equations

$$\tau_\nu = \frac{c^2}{8\pi\nu^2} A_{ij} N_u \exp\left(\frac{h\nu}{k_B T_{ex}}\right)$$

$$N_u = N_{tot} \frac{g_u}{Q} \exp\left(\frac{-E_u}{k_B T_{ex}}\right)$$

based on Equation 29 of Mangum & Shirley 2015 (2015PASP..127..266M)

pyspeckit.spectrum.models.lte\_molecule.**line\_tau\_cgs**(*tex*, *total\_column*, *partition\_function*, *degeneracy*, *frequency*, *energy\_upper*, *einstein\_A*)

Given the excitation temperature of the state, total column density of the molecule, the partition function, the degeneracy of the state, the frequency of the state, and the upper-state energy level, return the optical depth of that transition.

Unlike **line\_tau()**, this function requires inputs in CGS units.

This is a helper function for the LTE molecule calculations. It implements the equations

$$\tau_\nu = \frac{c^2}{8\pi\nu^2} A_{ij} N_u \exp\left(\frac{h\nu}{k_B T_{ex}}\right)$$

$$N_u = N_{tot} \frac{g_u}{Q} \exp\left(\frac{-E_u}{k_B T_{ex}}\right)$$

based on Equations 11 and 29 of Mangum & Shirley 2015 (2015PASP..127..266M)

### 3.2.4 Hyperfine Model

The hyperfine line modeling tool is a generic tool for modeling hyperfine lines. Given a list of hyperfine line separations and weights, it will treat the full set of lines as a single component when fitting. There are many options for the free parameters, as illustrated below:

#### Module API

```
class pyspeckit.spectrum.models.hyperfine.hyperfinemodel(line_names,          voff_lines_dict,
                                                         freq_dict,   line_strength_dict,  rela-
                                                         tive_strength_total_degeneracy)
```

Wrapper for the hyperfine model class. Specify the offsets and relative strengths when initializing, then you've got yourself a hyperfine modeler.

There are a wide variety of different fitter attributes, each designed to free a different subset of the parameters. Their purposes should be evident from their names.

Initialize the various parameters defining the hyperfine transitions

#### Parameters

##### **line\_names: list**

list of the line names to be used as indices for the dictionaries

##### **voff\_lines\_dict: dict**

a linename:v\_off dictionary of velocity offsets for the hyperfine components. Technically, this is redundant with freq\_dict

##### **freq\_dict: dict**

frequencies of the individual transitions

##### **line\_strength\_dict: dict**

Relative strengths of the hyperfine components, usually determined by their degeneracy and Einstein A coefficients

```
hyperfine(xarr, Tex=5.0, tau=0.1, xoff_v=0.0, width=1.0, return_hyperfine_components=False, Tback-
ground=2.73, amp=None, return_tau=False, tau_total=None, vary_hyperfine_tau=False,
vary_hyperfine_width=False)
```

Generate a model spectrum given an excitation temperature, optical depth, offset velocity, and velocity width.

#### Parameters

##### **return\_tau**

[bool] If specified, return just the tau spectrum, ignoring Tex

##### **tau\_total**

[bool] If specified, use this *instead of tau*, and it tries to normalize to the *peak of the line*

##### **vary\_hyperfine\_tau**

[bool] If set to true, allows the hyperfine transition amplitudes to vary and does not use the line\_strength\_dict. If set, tau must be a dict

```
hyperfine_addbackground(xarr, Tbackground=2.73, Tex=5.0, tau=0.1, xoff_v=0.0, width=1.0, re-
turn_tau=False, **kwargs)
```

Identical to hyperfine, but adds Tbackground as a constant continuum level

**hyperfine\_amp**(*xarr*, *amp=None*, *xoff\_v=0.0*, *width=1.0*, *return\_hyperfine\_components=False*, *Tbackground=2.73*, *Tex=5.0*, *tau=0.1*)  
wrapper of self.hyperfine with order of arguments changed

**hyperfine\_background**(*xarr*, *Tbackground=2.73*, *Tex=5.0*, *tau=0.1*, *xoff\_v=0.0*, *width=1.0*, *return\_tau=False*, *\*\*kwargs*)  
Identical to hyperfine, but with Tbackground free. Assumes already background-subtracted

**hyperfine\_tau**(*xarr*, *tau*, *xoff\_v*, *width*, *\*\*kwargs*)  
same as hyperfine, but with arguments in a different order, AND tau is returned instead of exp(-tau)

**hyperfine\_tau\_total**(*xarr*, *tau\_total*, *xoff\_v*, *width*, *\*\*kwargs*)  
same as hyperfine, but with arguments in a different order, AND tau is returned instead of exp(-tau), AND the *peak* tau is used

**hyperfine\_varyhf**(*xarr*, *Tex*, *xoff\_v*, *width*, *\*args*, *\*\*kwargs*)  
Wrapper of hyperfine for using a variable number of peaks with specified tau

**hyperfine\_varyhf\_amp**(*xarr*, *xoff\_v*, *width*, *\*args*, *\*\*kwargs*)  
Wrapper of hyperfine for using a variable number of peaks with specified amplitude (rather than tau). Uses some opaque tricks: Tex is basically ignored, and return\_tau means you're actually returning the amplitude, which is just passed in as tau

**hyperfine\_varyhf\_amp\_width**(*xarr*, *xoff\_v*, *\*args*, *\*\*kwargs*)  
Wrapper of hyperfine for using a variable number of peaks with specified amplitude (rather than tau). Uses some opaque tricks: Tex is basically ignored, and return\_tau means you're actually returning the amplitude, which is just passed in as tau

### 3.2.5 Model Grid

Fit a line based on parameters output from a grid of models

#### Module API

pyspeckit.spectrum.models.modelgrid.**gaussian\_line**(*xax*, *maxamp*, *tau*, *offset*, *width*)

A Gaussian line function in which the

pyspeckit.spectrum.models.modelgrid.**line\_model\_2par**(*xax*, *center*, *width*, *gridval1*, *gridval2*, *griddim1*, *griddim2*, *maxampgrid*, *taugrid*, *linefunction=<function gaussian\_line>*)

Returns the spectral line that matches the given x-axis

*xax*, *center*, *width* must be in the same units!

pyspeckit.spectrum.models.modelgrid.**line\_params\_2D**(*gridval1*, *gridval2*, *griddim1*, *griddim2*, *valuegrid*)

Given a 2D grid of modeled line values - the amplitude, e.g. excitation temperature, and the optical depth, tau - return the model spectrum

*griddims* contains the names of the axes and their values. . . it should have the same number of entries as *gridpars*

### 3.2.6 Spectral Template Model

#### Spectral Template Fitter

A tool to find the optimal shift and scaling for a given template model.

## Module API

`pyspeckit.spectrum.models.template.spectral_template_generator(template_spectrum, xshift_units='km/s', left=0, right=0)`

Given a `spectral_template`, return a model function with scale and shift as free parameters.

### Parameters

**template\_spectrum:** 'pyspeckit.spectrum.classes.Spectrum'

The template spectrum to fit

**xshift\_units:** str

The units of the shift parameter

**left/right:** float

The left and right edge parameters used for extrapolating outside the template if the template is smaller than the input spectrum. These cannot be NaN.

### Returns

**spectral\_template:** function

The model function that interpolates the template onto the given X-axis

`pyspeckit.spectrum.models.template.template_fitter(template_spectrum, xshift_units='km/s')`

Generator for Spectral Template fitter class

### Parameters

**template\_spectrum**

[pyspeckit.Spectrum] A valid spectrum to be scaled and shifted to match the input

**xshift\_units**

[str in pyspeckit.units.unit\_type\_dict] The units of the shift to fit. If you're using a velocity unit, make sure there's a reference X-unit for both the template spectrum and the input spectrum.

## Examples

```
>>> template = pyspeckit.Spectrum("template_spectrum.fits")
>>> dataspec = pyspeckit.Spectrum("DataSpectrum.fits")
>>> template_fitter = pyspeckit.models.template_fitter(template,
...                                                    xshift_units='angstroms')
>>> dataspec.Registry.add_fitter('template', template_fitter, 2)
>>> dataspec.specfit(fittype='template', guesses=[1,0])
>>> print dataspec.specfit.parinfo
```

## 3.3 Specific Models

### 3.3.1 Ammonia Models

The Ammonia modeling tools include a set of constants in the `ammonia_constants` module and the following ammonia modeling tools listed below.

There is also an ammonia fitter wrapper; see [Wrappers](#).

Note that there are two modules described here: the multi-rotational-transition fitter, which has its own set of custom functions, and a generic hyperfine-line fitting module meant to fit a single metastable (or non-metastable) transition.

Ammonia inversion transition TROT fitter translated from Erik Rosolowsky's <http://svn.ok.ubc.ca/svn/signals/nh3fit/>

## Module API

```
pyspeckit.spectrum.models.ammonia.ammonia(xarr,   trot=20,   tex=None,   ntot=14,   width=1,
                                             xoff_v=0.0,   fortho=0.0,   tau=None,   fill-
                                             ingfraction=None,   return_tau=False,   re-
                                             turn_tau_profile=False,   background_tb=2.7315,   ver-
                                             bose=False,   return_components=False,   debug=False,
                                             line_names=['oneone', 'twotwo', 'threethree', 'fourfour',
                                                         'fivefive', 'sixsix', 'sevenseven', 'eighteight', 'ninenine'])
```

Generate a model Ammonia spectrum based on input temperatures, column, and gaussian parameters

### Parameters

**xarr:** 'pyspeckit.spectrum.units.SpectroscopicAxis'

Array of wavelength/frequency values

**trot:** float

The rotational temperature of the lines. This is the excitation temperature that governs the relative populations of the rotational states.

**tex:** float or None

Excitation temperature. Assumed LTE if unspecified (None) or if  $\text{tex} > \text{trot}$ . This is the excitation temperature for *all* of the modeled lines, which means we are explicitly assuming  $T_{\text{ex}}$  is the same for all lines.

**ntot:** float

Total log column density of NH<sub>3</sub>. Can be specified as a float in the range 5-25

**width:** float

Line width in km/s

**xoff\_v:** float

Line offset in km/s

**fortho:** float

Fraction of NH<sub>3</sub> molecules in ortho state. Default assumes all para (fortho=0).

**tau:** None or float

If tau (optical depth in the 1-1 line) is specified, ntot is NOT fit but is set to a fixed value. The optical depths of the other lines are fixed relative to tau\_oneone

**fillingfraction:** None or float

fillingfraction is an arbitrary scaling factor to apply to the model

**return\_tau:** bool

Return a dictionary of the optical depths in each line instead of a synthetic spectrum

**return\_tau\_profile:** bool

Return a dictionary of the optical depth profiles in each line, i.e., the optical depths that will be used in conjunction with  $T_{\text{ex}}$  to produce the synthetic spectrum

**return\_components:** bool

Return a list of arrays, one for each hyperfine component, instead of just one array

**background\_tb**

[float] The background brightness temperature. Defaults to TCMB.

**verbose: bool**

More messages

**debug: bool**

For debugging.

**Returns****spectrum: 'numpy.ndarray'**

Synthetic spectrum with same shape as xarr

**component\_list: list**

List of `numpy.ndarray`'s, one for each hyperfine component

**tau\_dict: dict**

Dictionary of optical depth values for the various lines (if return\_tau is set)

```
class pyspeckit.spectrum.models.ammonia.ammonia_model(npeaks=1, npars=6, parnames=['trot',
                                         'tex', 'ntot', 'width', 'xoff_v', 'fortho'],
                                         **kwargs)
```

**The basic Ammonia (NH3) model with 6 free parameters:**

Trot, Tex, ntot, width, xoff\_v, and fortho

Trot is the rotational temperature. It governs the relative populations of the rotational states, i.e., the relative strength of different transitions

Tex is the excitation temperature. It is assumed constant across all states, which is not always a good assumption - a radiative transfer and excitation model is required to constrain this, though.

ntot is the total column density of p-NH3 integrated over all states.

width is the linewidth

xoff\_v is the velocity offset / line of sight velocity

fortho is the ortho fraction (northo / (northo+npara))

**annotations()**

Return a list of TeX-formatted labels

The values and errors are formatted so that only the significant digits are displayed. Rounding is performed using the decimal package.

**Parameters****shortvarnames**

[list] A list of variable names (tex is allowed) to include in the annotations. Defaults to self.shortvarnames

**Examples**

```
>>> # Annotate a Gaussian
>>> sp.specfit.annotate(shortvarnames=['A', '\Delta x', '\sigma'])
```

**components**(*xarr, pars, hyperfine=False, return\_hyperfine\_components=False, \*\*kwargs*)

Ammonia components don't follow the default, since in Galactic astronomy the hyperfine components should be well-separated. If you want to see the individual components overlaid, you'll need to pass `hyperfine` to the `plot_fit` call

**moments**(*Xax, data, negamp=None, veryverbose=False, \*\*kwargs*)

Returns a very simple and likely incorrect guess

**multinh3fit**(*xax, data, err=None, parinfo=None, quiet=True, shh=True, debug=False, maxiter=200, use\_lmfit=False, veryverbose=False, \*\*kwargs*)

Fit multiple nh3 profiles (multiple can be 1)

### Parameters

#### **xax**

[array] x axis

#### **data**

[array] y axis

#### **npeaks**

[int] How many nh3 profiles to fit? Default 1 (this could supersede `onedgaussfit`)

#### **err**

[array] error corresponding to data

#### **params**

[list] Fit parameters: [trot, tex, ntot (or tau), width, offset, ortho fraction] \* npeaks If `len(params) % 6 == 0`, npeaks will be set to `len(params) / 6`. These parameters (and the related fixed, limited, min/max, names below) need to have length = `6*npeaks`. If npeaks > 1 and length = 6, they will be replicated npeaks times, otherwise they will be reset to defaults:

#### **fixed**

[list] Is parameter fixed?

#### **limitedmin**

[list]

#### **minpars**

[list] set lower limits on each parameter (default: width>0, Tex and trot > Tcmb)

#### **limitedmax**

[list]

#### **maxpars**

[list] set upper limits on each parameter

#### **parnames**

[list] default parameter names, important for setting kwargs in model  
['trot','tex','ntot','width','xoff\_v','fortho']

#### **quiet**

[bool] should MPFIT output each iteration?

#### **shh**

[bool] output final parameters?

### Returns



**mpp**  
[model parameter object] Fit parameters

**model**  
[array] The model array

**errors**  
[array] the fit errors

**chi2**  
[float] the  $\chi^2$  value of the fit

**n\_ammonia**(*pars=None, parnames=None, \*\*kwargs*)

Returns a function that sums over N ammonia line profiles, where N is the length of *trot, tex, ntot, width, xoff\_v, fortho* OR  $N = \text{len}(\text{pars}) / 6$

The background “height” is assumed to be zero (you must “baseline” your spectrum before fitting)

**pars** [ list ]  
a list with  $\text{len}(\text{pars}) = (6 - n_{\text{fixed}})n$ , assuming *trot, tex, ntot, width, xoff\_v, fortho* repeated

**parnames** [ list ]  
 $\text{len}(\text{parnames})$  must =  $\text{len}(\text{pars})$ . *parnames* determine how the ammonia function parses the arguments

**parse\_3par\_guesses**(*guesses*)

Try to convert a set of interactive guesses (peak, center, width) into guesses appropriate to the model.

**For NH3 models, we add in several extra parameters:**

$\text{tex} = 2.73 * \text{peak}$   $\text{trot} = \text{tex} * 2$   $\text{fortho} = 0.5$   $\text{ntot} = 15$

*ntot* is set to a constant  $\sim 10^{15}$  because this results in optical depths near 1, so it forces the emission to be approximately significant.  $\text{trot} > \text{tex}$  so that we’re in a physical regime to begin with.

We assume  $\text{tex} = \text{peak} + 2.73$  because most spectra are shown background-subtracted (single dish are always that way, interferometric data are intrinsically that way...) and otherwise the guessing will crash if you guess a number  $< 2.73$ .

**class** pyspeckit.spectrum.models.ammonia.**ammonia\_model\_background**(*\*\*kwargs*)

**moments**(*Xax, data, negamp=None, veryverbose=False, \*\*kwargs*)

Returns a very simple and likely incorrect guess

**multinh3fit**(*xax, data, npeaks=1, err=None, params=(20, 20, 14, 1.0, 0.0, 0.5, 2.7315), parnames=None, fixed=(False, False, False, False, False, False, True), limitedmin=(True, True, True, False, True, True), limitedmax=(False, False, False, False, False, True, True), minpars=(2.7315, 2.7315, 0, 0, 0, 0, 2.7315), parinfo=None, maxpars=(0, 0, 0, 0, 0, 1, 2.7315), tied=(", ", ", ", ", ", ", ), quiet=True, shh=True, veryverbose=False, \*\*kwargs*)  
Fit multiple nh3 profiles (multiple can be 1)

**Parameters**

**xax**  
[array] x axis

**data**  
[array] y axis

**npeaks**  
[int] How many nh3 profiles to fit? Default 1 (this could supersede onedgaussfit)

**err**  
[array] error corresponding to data

**params**

[list] Fit parameters: [trot, tex, ntot (or tau), width, offset, ortho fraction] \* npeaks If len(params) % 6 == 0, npeaks will be set to len(params) / 6. These parameters (and the related fixed, limited, min/max, names below) need to have length = 6\*npeaks. If npeaks > 1 and length = 6, they will be replicated npeaks times, otherwise they will be reset to defaults:

**fixed**

[list] Is parameter fixed?

**limitedmin**

[list]

**minpars**

[list] set lower limits on each parameter (default: width>0, Tex and trot > Tcmb)

**limitedmax**

[list]

**maxpars**

[list] set upper limits on each parameter

**parnames**

[list] default parameter names, important for setting kwargs in model  
[‘trot’, ‘tex’, ‘ntot’, ‘width’, ‘xoff\_v’, ‘fortho’]

**quiet**

[bool] should MPFIT output each iteration?

**shh**

[bool] output final parameters?

**Returns****mpp**

[model parameter object] Fit parameters

**model**

[array] The model array

**errors**

[array] the fit errors

**chi2**

[float] the chi<sup>2</sup> value of the fit

```
class pyspeckit.spectrum.models.ammonia.ammonia_model_restricted_tex(parnames=[‘trot’, ‘tex’,
                                                                              ‘ntot’, ‘width’, ‘xoff_v’,
                                                                              ‘fortho’, ‘delta’],
                                                                              **kwargs)
```

```
make_parinfo(params=(20, 20, 0.5, 1.0, 0.0, 0.5, 0), fixed=(False, False, False, False, False, False,
False), limitedmin=(True, True, True, True, False, True, True), limitedmax=(False, False,
False, False, False, True, False), minpars=(2.7315, 2.7315, 0, 0, 0, 0, 0), maxpars=(0, 0,
0, 0, 0, 1, 0), tied=(“, ‘p[0]-p[6]’, “, “, “, “, “), **kwargs)
parnames=[‘trot’, ‘tex’, ‘ntot’, ‘width’, ‘xoff_v’, ‘fortho’, ‘delta’]
```

‘delta’ is the difference between tex and trot

**n\_ammonia**(*pars=None, parnames=None, \*\*kwargs*)

Returns a function that sums over N ammonia line profiles, where N is the length of *trot, tex, ntot, width, xoff\_v, fortho* OR  $N = \text{len}(\text{pars}) / 6$

The background “height” is assumed to be zero (you must “baseline” your spectrum before fitting)

**pars** [ list ]

a list with  $\text{len}(\text{pars}) = (6 - n_{\text{fixed}})n$ , assuming *trot, tex, ntot, width, xoff\_v, fortho* repeated

**parnames** [ list ]

$\text{len}(\text{parnames}) \text{ must } = \text{len}(\text{pars})$ . *parnames* determine how the ammonia function parses the arguments

```
class pyspeckit.spectrum.models.ammonia.ammonia_model_vtau(parnames=['trot', 'tex', 'tau',
                                'width', 'xoff_v', 'fortho'],
                                **kwargs)
```

```
make_parinfo(params=(20, 14, 0.5, 1.0, 0.0, 0.5), fixed=(False, False, False, False, False, False), lim-
itedmin=(True, True, True, True, False, True), limitedmax=(False, False, False, False,
False, True), minpars=(2.7315, 2.7315, 0, 0, 0, 0), maxpars=(0, 0, 0, 0, 0, 1), tied=(", "
", ", ", ", "), **kwargs)
parnames=['trot', 'tex', 'tau', 'width', 'xoff_v', 'fortho']
```

**moments**(*Xax, data, negamp=None, veryverbose=False, \*\*kwargs*)

Returns a very simple and likely incorrect guess

```
class pyspeckit.spectrum.models.ammonia.ammonia_model_vtau_thin(parnames=['tkin', 'tau',
                                'width', 'xoff_v', 'fortho'],
                                **kwargs)
```

```
make_parinfo(params=(20, 14, 1.0, 0.0, 0.5), fixed=(False, False, False, False, False), limited-
min=(True, True, True, False, True), limitedmax=(False, False, False, False, True), min-
pars=(2.7315, 0, 0, 0, 0, 0), maxpars=(0, 0, 0, 0, 0, 1), tied=(", ", ", ", ", ", "), **kwargs)
parnames=['trot', 'tex', 'tau', 'width', 'xoff_v', 'fortho']
```

**moments**(*Xax, data, negamp=None, veryverbose=False, \*\*kwargs*)

Returns a very simple and likely incorrect guess

```
pyspeckit.spectrum.models.ammonia.ammonia_thin(xarr, tkin=20, tex=None, ntot=14, width=1,
xoff_v=0.0, fortho=0.0, tau=None, re-
turn_tau=False, **kwargs)
```

Use optical depth in the 1-1 line as a free parameter The optical depths of the other lines are then set by the kinetic temperature

*tkin* is used to compute *trot* assuming a 3-level system consisting of (1,1), (2,1), and (2,2) as in Swift et al, 2005 [2005ApJ...620..823S]

```
pyspeckit.spectrum.models.ammonia.cold_ammonia(xarr, tkin, **kwargs)
```

Generate a model Ammonia spectrum based on input temperatures, column, and gaussian parameters

### Parameters

**xarr:** ‘pyspeckit.spectrum.units.SpectroscopicAxis’

Array of wavelength/frequency values

**tkin:** float

The kinetic temperature of the lines in K. Will be converted to rotational temperature following the scheme of Swift et al 2005 (<http://esoads.eso.org/abs/2005ApJ...620..823S>, eqn A6) and further discussed in Equation 7 of Rosolowsky et al 2008 (<http://adsabs.harvard.edu/abs/2008ApJS..175..509R>)

```
class pyspeckit.spectrum.models.ammonia.cold_ammonia_model(parnames=['tkin', 'tex', 'ntot',
                                                                    'width', 'xoff_v', 'fortho'],
                                                            **kwargs)
```

### Ammonia inversion transition: Hyperfine-only fitter

#### Module API

pyspeckit.spectrum.models.ammonia\_hf.nh3\_vtau\_multimodel\_generator(linenames)

If you want to use multiple hyperfines for the same spectrum, use this generator. It is useful if you want N independent tau/tex values but the same velocity and linewidth

#### Parameters

##### linenames

[list] A list of line names from the set ('oneone', ..., 'eighteight')

#### Returns

##### model

[model.SpectralModel] A SpectralModel class build from N different metastable inversion hyperfine models

### 3.3.2 Formaldehyde Models

The Formaldehyde model is based on the [Hyperfine Model](#). There is also a mm-line fitting module that uses preconstructed model grids to fit temperature from multiple transitions.

There is a formaldehyde fitter wrapper; see [Wrappers](#).

This is a formaldehyde 1<sub>11</sub>-1<sub>10</sub> / 2<sub>12</sub>-2<sub>11</sub> fitter. It includes hyperfine components of the formaldehyde lines and has both LTE and RADEX LVG based models

#### Module API

```
pyspeckit.spectrum.models.formaldehyde.formaldehyde(xarr, amp=1.0, xoff_v=0.0, width=1.0,
                                                       return_hypfine_components=False, texs-
                                                       cale=0.01, tau=0.01, **kwargs)
```

Generate a model Formaldehyde spectrum based on simple gaussian parameters

the “amplitude” is an essentially arbitrary parameter; we therefore define it to be Tex given tau=0.01 when passing to the fitter The final spectrum is then rescaled to that value

```
class pyspeckit.spectrum.models.formaldehyde.formaldehyde_model(modelfunc, npars, short-
                                                                    varnames=('A', '\Delta x',
                                                                    '\sigma'), fitunit=None,
                                                                    centroid_par=None,
                                                                    fwhm_func=None,
                                                                    fwhm_pars=None, in-
                                                                    tegral_func=None,
                                                                    use_lmfit=False,
                                                                    guess_types=('amplitude',
                                                                    'center', 'width'), **kwargs)
```

Spectral Model Initialization

Create a Spectral Model class for data fitting

### Parameters

**modelfunc**

[function] the model function to be fitted. Should take an X-axis (spectroscopic axis) as an input followed by input parameters. Returns an array with the same shape as the input X-axis

**npars**

[int] number of parameters required by the model

**parnames**

[list (optional)] a list or tuple of the parameter names

**parvalues**

[list (optional)] the initial guesses for the input parameters (defaults to ZEROS)

**parlimits**

[list (optional)] the upper/lower limits for each variable (defaults to ZEROS)

**parfixed**

[list (optional)] Can declare any variables to be fixed (defaults to ZEROS)

**parerror**

[list (optional)] technically an output parameter. Specifying it here will have no effect. (defaults to ZEROS)

**partied**

[list (optional)] not the past tense of party. Can declare, via text, that some parameters are tied to each other. Defaults to zeros like the others, but it's not clear if that's a sensible default

**fitunit**

[str (optional)] convert X-axis to these units before passing to model

**parsteps**

[list (optional)] minimum step size for each parameter (defaults to ZEROS)

**npeaks**

[list (optional)] default number of peaks to assume when fitting (can be overridden)

**shortvarnames**

[list (optional)] TeX names of the variables to use when annotating

**amplitude\_types**

[tuple] A tuple listing the types of the different parameters when guessing. The valid values are 'amplitude', 'width', and 'center'. These are handled by `parse_3par_guesses`, which translate these into input guess lists for the fitter. For a "standard" 3-parameter Gaussian fitter, nothing changes, but for other models that have more than 3 parameters, some translation is needed.

### Returns

A tuple containing (model best-fit parameters, the model, parameter

errors,  $\chi^2$  value)

**formaldehyde\_integral**(*modelpars*, *linename*='oneone')

Return the integral of the individual components (ignoring height)

`pyspeckit.spectrum.models.formaldehyde.formaldehyde_pyradex(xarr, density=4, column=13, temperature=20, xoff_v=0.0, opr=1.0, width=1.0, tbackground=2.73, grid_vwidth=1.0, debug=False, verbose=False, **kwargs)`

Use a grid of RADEX-computed models to make a model line spectrum

The RADEX models have to be available somewhere. OR they can be passed as arrays. If as arrays, the form should be: `texgrid = ((minfreq1,maxfreq1,texgrid1),(minfreq2,maxfreq2,texgrid2))`

`xarr` must be a `SpectroscopicAxis` instance `xoff_v`, `width` are both in km/s

`grid_vwidth` is the velocity assumed when computing the grid in km/s this is important because  $\tau = \text{modeltau} / \text{width}$  (see, e.g., Draine 2011 textbook pgs 219-230)

`pyspeckit.spectrum.models.formaldehyde.formaldehyde_radex(xarr, density=4, column=13, xoff_v=0.0, width=1.0, grid_vwidth=1.0, grid_vwidth_scale=False, texgrid=None, taugrid=None, hdr=None, path_to_texgrid="", path_to_taugrid="", temperature_gridnumber=3, debug=False, verbose=False, **kwargs)`

Use a grid of RADEX-computed models to make a model line spectrum

The RADEX models have to be available somewhere. OR they can be passed as arrays. If as arrays, the form should be: `texgrid = ((minfreq1,maxfreq1,texgrid1),(minfreq2,maxfreq2,texgrid2))`

`xarr` must be a `SpectroscopicAxis` instance `xoff_v`, `width` are both in km/s

`grid_vwidth` is the velocity assumed when computing the grid in km/s this is important because  $\tau = \text{modeltau} / \text{width}$  (see, e.g., Draine 2011 textbook pgs 219-230) `grid_vwidth_scale` is True or False: False for LVG, True for Sphere

`pyspeckit.spectrum.models.formaldehyde.formaldehyde_radex_orthopara_temp(xarr, density=4, column=13, orthopara=1.0, temperature=15.0, xoff_v=0.0, width=1.0, Tbackground1=2.73, Tbackground2=2.73, grid_vwidth=1.0, grid_vwidth_scale=False, texgrid=None, taugrid=None, hdr=None, path_to_texgrid="", path_to_taugrid="", debug=False, verbose=False, getpars=False, **kwargs)`

Use a grid of RADEX-computed models to make a model line spectrum

The RADEX models have to be available somewhere. OR they can be passed as arrays. If as arrays, the form should be: `texgrid = ((minfreq1,maxfreq1,texgrid1),(minfreq2,maxfreq2,texgrid2))`

`xarr` must be a `SpectroscopicAxis` instance `xoff_v`, `width` are both in km/s

`grid_vwidth` is the velocity assumed when computing the grid in km/s this is important because  $\tau = \text{modeltau} / \text{width}$  (see, e.g., Draine 2011 textbook pgs 219-230) `grid_vwidth_scale` is True or False: False for LVG, True for Sphere

```
pyspeckit.spectrum.models.formaldehyde.formaldehyde_radex_tau(xarr,      density=4,      col-
                                                                umn=13,      xoff_v=0.0,
                                                                width=1.0,      grid_vwidth=1.0,
                                                                grid_vwidth_scale=False,
                                                                taugrid=None,      hdr=None,
                                                                path_to_taugrid="",      tem-
                                                                perature_gridnumber=3,      de-
                                                                bug=False,      verbose=False,      re-
                                                                turn_hyperfine_components=False,
                                                                **kwargs)
```

Use a grid of RADEX-computed models to make a model line spectrum

- uses hyperfine components
- assumes *tau* varies but *tex* does not!

The RADEX models have to be available somewhere. OR they can be passed as arrays. If as arrays, the form should be: `texgrid = ((minfreq1,maxfreq1,texgrid1),(minfreq2,maxfreq2,texgrid2))`

`xarr` must be a `SpectroscopicAxis` instance `xoff_v`, `width` are both in km/s

`grid_vwidth` is the velocity assumed when computing the grid in km/s this is important because  $\tau = \text{modeltau} / \text{width}$  (see, e.g., Draine 2011 textbook pgs 219-230) `grid_vwidth_scale` is True or False: False for LVG, True for Sphere

This is a formaldehyde 3\_03-2\_02 / 3\_22-221 and 3\_03-2\_02/3\_21-2\_20 fitter. It is based entirely on RADEX models.

## Module API

```
pyspeckit.spectrum.models.formaldehyde_mm.build_despotic_grids(gridfile='ph2co_grid_despotic.fits',
                                                                ph2coAbund=1e-08, nDens=21,
                                                                logDensLower=2.0,      log-
                                                                DensUpper=6.0,      nCol=21,
                                                                logColLower=11.0,      log-
                                                                ColUpper=15.0,      nTemp=51,
                                                                Tlower=10.0,      Tupper=300.0,
                                                                nDv=5,      DvLower=1.0,      DvUp-
                                                                per=5.0)
```

Generates grids of p-H<sub>2</sub>CO line intensities using Despotic. Outputs a `astropy Table`.

### Parameters

#### **gridfile**

[string] Name of grid file to output.

#### **ph2coAbund**

[float] Fractional abundance of p-H<sub>2</sub>CO

#### **nDens**

[int] Number of grid points in the volume density

**logDensLower**

[float] log of volume density at lower bound of grid ( $\log(n/\text{cm}^{-3})$ )

**logDensUpper**

[float] log of volume density at upper bound of grid ( $\log(n/\text{cm}^{-3})$ )

**nCol**

[int] Number of grid points in the column density

**logColLower**

[float] log of column density of p-H<sub>2</sub>CO at lower bound of grid ( $\log(N/\text{cm}^{-2})$ )

**logColUpper**

[float] log of column density of p-H<sub>2</sub>CO at upper bound of grid ( $\log(N/\text{cm}^{-2})$ )

**nTemp**

[int] Number of grid points in the temperature grid

**Tower**

[float] temperature at lower bound of grid (K)

**Tupper**

[float] temperature at upper bound of grid (K)

**nDv**

[int] Number of grid points in the line width

**DvLower**

[float] line width (non-thermal) at lower bound of grid (km/s)

**DvUpper**

[float] line width (non-thermal) at upper bound of grid (km/s)

```
pyspeckit.spectrum.models.formaldehyde_mm.formaldehyde_mm(xarr, amp=1.0, xoff_v=0.0, width=1.0,
                                                             return_components=False)
```

Generate a model Formaldehyde spectrum based on simple gaussian parameters

the “amplitude” is an essentially arbitrary parameter; we therefore define it to be Tex given tau=0.01 when passing to the fitter The final spectrum is then rescaled to that value

The components are independent, but with offsets set by frequency... in principle.

```
pyspeckit.spectrum.models.formaldehyde_mm.formaldehyde_mm_despotic(xarr,      temperature=25,
                                                                    column=13,    density=4,
                                                                    xoff_v=0.0,   width=1.0,
                                                                    grid_vwidth=1.0,
                                                                    h2co_303_202=None,
                                                                    h2co_322_221=None,
                                                                    h2co_321_220=None, de-
                                                                    bug=False, verbose=False,
                                                                    **kwargs)
```

Fitter to p-H<sub>2</sub>CO using despotic grids. Requires building grids and passing in functions for interpolating the h2co transition optical depth and excitation temperatures.

```
pyspeckit.spectrum.models.formaldehyde_mm.formaldehyde_mm_despotic_functions(gridtable)
```

This builds interpolation functions for use in fitting.

**Parameters****gridtable**

[str] Name of grid in astropy table



## Returns

### **h2co\_303\_202, h2co\_322\_221, h2co\_321\_220**

[function] Functions that return the excitation temperature and optical depth given input density, temperature, column density and line width.

```
class pyspeckit.spectrum.models.formaldehyde_mm.formaldehyde_mm_model(modelfunc,      npars,
                                                                    shortvarnames=('A',
                                                                    '\Delta x',  '\sigma'),
                                                                    fitunit=None,      cen-
                                                                    troid_par=None,
                                                                    fwhm_func=None,
                                                                    fwhm_pars=None,
                                                                    integral_func=None,
                                                                    use_lmfit=False,
                                                                    guess_types=('amplitude',
                                                                    'center',    'width'),
                                                                    **kwargs)
```

Spectral Model Initialization

Create a Spectral Model class for data fitting

## Parameters

### **modelfunc**

[function] the model function to be fitted. Should take an X-axis (spectroscopic axis) as an input followed by input parameters. Returns an array with the same shape as the input X-axis

### **npars**

[int] number of parameters required by the model

### **parnames**

[list (optional)] a list or tuple of the parameter names

### **parvalues**

[list (optional)] the initial guesses for the input parameters (defaults to ZEROS)

### **parlimits**

[list (optional)] the upper/lower limits for each variable (defaults to ZEROS)

### **parfixed**

[list (optional)] Can declare any variables to be fixed (defaults to ZEROS)

### **parerror**

[list (optional)] technically an output parameter. Specifying it here will have no effect. (defaults to ZEROS)

### **partied**

[list (optional)] not the past tense of party. Can declare, via text, that some parameters are tied to each other. Defaults to zeros like the others, but it's not clear if that's a sensible default

### **fitunit**

[str (optional)] convert X-axis to these units before passing to model

### **parsteps**

[list (optional)] minimum step size for each parameter (defaults to ZEROS)

**npeaks**

[list (optional)] default number of peaks to assume when fitting (can be overridden)

**shortvarnames**

[list (optional)] TeX names of the variables to use when annotating

**amplitude\_types**

[tuple] A tuple listing the types of the different parameters when guessing. The valid values are 'amplitude', 'width', and 'center'. These are handled by `parse_3par_guesses`, which translate these into input guess lists for the fitter. For a "standard" 3-parameter Gaussian fitter, nothing changes, but for other models that have more than 3 parameters, some translation is needed.

**Returns**

A tuple containing (model best-fit parameters, the model, parameter

errors,  $\chi^2$  value)

```
pyspeckit.spectrum.models.formaldehyde_mm.formaldehyde_mm_radex(xarr,          temperature=25,
                                                                    column=13,          density=4,
                                                                    xoff_v=0.0,         width=1.0,
                                                                    grid_vwidth=1.0,    tex-
                                                                    grid=None,          tau-
                                                                    grid=None,          hdr=None,
                                                                    path_to_texgrid="",
                                                                    path_to_taugrid="", debug=False, verbose=False,
                                                                    **kwargs)
```

Use a grid of RADEX-computed models to make a model line spectrum

The RADEX models have to be available somewhere. OR they can be passed as arrays. If as arrays, the form should be: `texgrid = ((minfreq1,maxfreq1,texgrid1),(minfreq2,maxfreq2,texgrid2))`

`xarr` must be a `SpectroscopicAxis` instance `xoff_v`, `width` are both in km/s

**Parameters****grid\_vwidth**

[float] the velocity assumed when computing the grid in km/s this is important because `tau = modeltau / width` (see, e.g., Draine 2011 textbook pgs 219-230)

**density**

[float] Density!

Erik R's "fork" of the mm fitter:

This is a formaldehyde 3\_03-2\_02 / 3\_22-221 and 3\_03-2\_02/3\_21-2\_20 fitter. It is based entirely on RADEX models.

This is the EWR fork of the fitter in `pyspeckit`.

**Module API**

```
pyspeckit.spectrum.models.h2co_mm.formaldehyde_mm(xarr, amp=1.0, xoff_v=0.0, width=1.0, re-
                                                                    turn_components=False)
```

Generate a model Formaldehyde spectrum based on simple gaussian parameters

the “amplitude” is an essentially arbitrary parameter; we therefore define it to be  $\text{Tex}$  given  $\tau=0.01$  when passing to the fitter. The final spectrum is then rescaled to that value.

The components are independent, but with offsets set by frequency... in principle.

```
class pyspeckit.spectrum.models.h2co_mm.formaldehyde_mm_model(modelfunc, npars, short-
                                                             varnames=('A', '\Delta x',
                                                             '\sigma'), fitunit=None,
                                                             centroid_par=None,
                                                             fwhm_func=None,
                                                             fwhm_pars=None, in-
                                                             tegral_func=None,
                                                             use_lmfit=False,
                                                             guess_types=('amplitude',
                                                             'center', 'width'), **kwargs)
```

Spectral Model Initialization

Create a Spectral Model class for data fitting

### Parameters

#### **modelfunc**

[function] the model function to be fitted. Should take an X-axis (spectroscopic axis) as an input followed by input parameters. Returns an array with the same shape as the input X-axis

#### **npars**

[int] number of parameters required by the model

#### **parnames**

[list (optional)] a list or tuple of the parameter names

#### **parvalues**

[list (optional)] the initial guesses for the input parameters (defaults to ZEROS)

#### **parlimits**

[list (optional)] the upper/lower limits for each variable (defaults to ZEROS)

#### **parfixed**

[list (optional)] Can declare any variables to be fixed (defaults to ZEROS)

#### **parerror**

[list (optional)] technically an output parameter. Specifying it here will have no effect. (defaults to ZEROS)

#### **partied**

[list (optional)] not the past tense of party. Can declare, via text, that some parameters are tied to each other. Defaults to zeros like the others, but it's not clear if that's a sensible default

#### **fitunit**

[str (optional)] convert X-axis to these units before passing to model

#### **parsteps**

[list (optional)] minimum step size for each parameter (defaults to ZEROS)

#### **npeaks**

[list (optional)] default number of peaks to assume when fitting (can be overridden)

#### **shortvarnames**

[list (optional)] TeX names of the variables to use when annotating

**amplitude\_types**

[tuple] A tuple listing the types of the different parameters when guessing. The valid values are 'amplitude', 'width', and 'center'. These are handled by `parse_3par_guesses`, which translate these into input guess lists for the fitter. For a "standard" 3-parameter Gaussian fitter, nothing changes, but for other models that have more than 3 parameters, some translation is needed.

**Returns**

**A tuple containing (model best-fit parameters, the model, parameter**

**errors, chi^2 value)**

```
pyspeckit.spectrum.models.h2co_mm.h2co_mm_radex(xarr, Temperature=25, logColumn=13, logDensity=4, xoff_v=0.0, width=1.0, grid_vwidth=1.0, gridbundle=None, debug=False, verbose=False, **kwargs)
```

Use a grid of RADEX-computed models to make a model line spectrum

The RADEX models have to be available somewhere. OR they can be passed as arrays. If as arrays, the form should be: `texgrid = ((minfreq1,maxfreq1,texgrid1),(minfreq2,maxfreq2,texgrid2))`

`xarr` must be a `SpectroscopicAxis` instance `xoff_v`, `width` are both in km/s

**Parameters****grid\_vwidth**

[float] the velocity assumed when computing the grid in km/s this is important because  $\tau = \text{modeltau} / \text{width}$  (see, e.g., Draine 2011 textbook pgs 219-230)

**density**

[float] Density!

### 3.3.3 HCN Model

HCN is a molecule with hyperfine lines. It uses the hyperfine wrapper.

This is an HCN fitter. . . ref for line params: <http://www.strw.leidenuniv.nl/~moldata/datafiles/hcn@hfs.dat>

**Module API**

```
pyspeckit.spectrum.models.hcn.aval_dict = {'10-01': 2.4075e-05, '11-01': 2.4075e-05, '12-01': 2.4075e-05}
```

Line strengths of the 15 hyperfine components in  $J = 1 - 0$  transition. The thickness of the lines indicates their relative weight compared to the others. Line strengths are normalized in such a way that summing over all initial  $J = 1$  levels gives the degeneracy of the  $J = 0$  levels, i.e., for  $JF1F = 012$ , three for  $JF1F = 011$ , and one for  $JF1F = 010$ . Thus, the sum over all 15 transitions gives the total spin degeneracy

```
pyspeckit.spectrum.models.hcn.hcn_radex(xarr, density=4, column=13, xoff_v=0.0, width=1.0, grid_vwidth=1.0, grid_vwidth_scale=False, texgrid=None, taugrid=None, hdr=None, path_to_texgrid="", path_to_taugrid="", temperature_gridnumber=3, debug=False, verbose=False, **kwargs)
```

Use a grid of RADEX-computed models to make a model line spectrum

The RADEX models have to be available somewhere. OR they can be passed as arrays. If as arrays, the form should be: `texgrid = ((minfreq1,maxfreq1,texgrid1),(minfreq2,maxfreq2,texgrid2))`

`xarr` must be a `SpectroscopicAxis` instance `xoff_v`, `width` are both in km/s

`grid_vwidth` is the velocity assumed when computing the grid in km/s this is important because  $\tau = \text{modeltau} / \text{width}$  (see, e.g., Draine 2011 textbook pgs 219-230) `grid_vwidth_scale` is True or False: False for LVG, True for Sphere

### 3.3.4 Hill5 Infall Model

The Hill5 infall model is a specific realization of a collapsing cloud profile.

Code translated from: [https://bitbucket.org/devries/analytic\\_infall/overview](https://bitbucket.org/devries/analytic_infall/overview)

Original source: <http://adsabs.harvard.edu/abs/2005ApJ...620..800D>

#### Module API

`pyspeckit.spectrum.models.hill5infall.hill5_model(xarr, tau, v_lsr, v_infall, sigma, tpeak, TBG=2.73)`

The hill5 from de Vries and Myers 2005. This model implicitly has zero optical depth in the envelope, no envelope velocity, and has a fixed background radiation temperature (see Table 2 in the paper).

#### Parameters

##### **xarr**

[np.ndarray] array of x values

##### **tau**

[float] `tau_c`, the core-center optical depth

##### **v\_lsr**

[float] The centroid velocity in km/s

##### **v\_infall**

[float] The infall velocity

##### **sigma**

[float] The line width

##### **tpeak**

[float] The peak brightness temperature

##### **TBG**

[float] The background temperature

`pyspeckit.spectrum.models.hill5infall.jfunc(t, nu)`  
*t*- kelvin *nu* - Hz?

### 3.3.5 N2H+ Model

#### N2H+ fitter

Reference for line params: Daniel, F., Dubernet, M.-L., Meuwly, M., Cernicharo, J., Pagani, L. 2005, MNRAS 363, 1083

<http://www.strw.leidenuniv.nl/~moldata/N2H+.html>

## Module API

Use a grid of RADEX-computed models to make a model line spectrum

xarr must be a SpectroscopicAxis instance xoff\_v, width are both in km/s

```
pyspeckit.spectrum.models.n2hp.relative_strength_total_degeneracy = {'101-010': 9.0, '101-011': 9.0, '101-012': 9.0,
```

Line strengths of the 15 hyperfine components in J=1-0 transition. The thickness of the lines indicates their relative weight compared to the others. Line strengths are normalized in such a way that summing over all initial J = 1 levels gives the degeneracy of the J = 0 levels, i.e., for JF1F 012, three for JF1F 011, and one for JF1F 010. Thus, the sum over all 15 transitions gives the total spin degeneracy

## Hydrogen Models

The values for the Case B recombination coefficients are given by [Hummer & Storey \(1987\)](#). They are also computed in [Hummer \(1994\)](#) and tabulated at a [wiki](#). I had to OCR and pull out by hand some of the coefficients.

## Module API

### Add the Hydrogen model to the Spectrum's fitter registry

Given a `pyspeckit.units.SpectroscopicAxis` instance, finds all the lines that are in bounds. Returns a list of line names.

Generate a set of parameters identifying the hydrogen lines in your spectrum. These come in groups of 3 assuming you're fitting a gaussian to each. You can tie the widths or choose not to.

The case B coefficients are computed for 3 temperatures

Should the widths be tied?

Returns a list of tied and guesses in the xarr's units

`pyspeckit.spectrum.models.hydrogen.hydrogen_model(xarr, amplitude=1.0, width=0.0, velocity=0.0, a_k=0.0, temperature=10000)`

Generate a set of parameters identifying the hydrogen lines in your spectrum. These come in groups of 3 assuming you're fitting a gaussian to each. You can tie the widths or choose not to.

#### Parameters

**sp**

[pyspeckit.Spectrum] The spectrum to fit

**temperature**

[[ 5000, 10000, 20000 ]] The case B coefficients are computed for 3 temperatures

**a\_k**

[float] The K-band extinction normalized to 2.2 microns. Simple exponential.

**width**

[float] Line width in km/s

**velocity**

[float] Line center in km/s

**amplitude**

[float] arbitrary amplitude of the first line (all other lines will be scaled to this value)

#### Returns

**np.ndarray with same shape as sp.xarr**

`pyspeckit.spectrum.models.hydrogen.rrl(n, dn=1, amu=1.007825, Z=1)`

compute Radio Recomb Line freqs in GHz from Brown, Lockman & Knapp ARAA 1978 16 445

#### UPDATED:

Gordon & Sorochenko 2009, eqn A6

#### Parameters

**n**

[int] The number of the lower level of the recombination line (H1a is Lyman alpha, for example)

**dn**

[int] The delta-N of the transition. alpha=1, beta=2, etc.

**amu**

[float] The mass of the central atom

**Z**

[int] The ionization parameter for the atom. Z=1 is neutral, Z=2 is singly ionized, etc. For hydrogen, only z=1 makes sense, since ionized hydrogen has no electrons and therefore cannot have recombination lines.

#### Returns

**frequency in GHz**

## 3.4 API Documentation for Models

We include the API documentation for the generic model and fitter wrappers here.

### 3.4.1 Module API

**class** pyspeckit.spectrum.models.model.**AstropyModel**(*model*, *shortvarnames=None*, *\*\*kwargs*)

Override the SpectralModel initialization

**fitter**(*xax*, *data*, *err=None*, *quiet=True*, *veryverbose=False*, *debug=False*, *parinfo=None*,  
*params=None*, *npeaks=None*, *\*\*kwargs*)

Run the fitter using mpfit.

kwargs will be passed to `_make_parinfo` and `mpfit`.

#### Parameters

##### **xax**

[SpectroscopicAxis] The X-axis of the spectrum

##### **data**

[ndarray] The data to fit

##### **err**

[ndarray (optional)] The error on the data. If unspecified, will be uniform unity

##### **parinfo**

[ParinfoList] The guesses, parameter limits, etc. See `pyspeckit.spectrum.parinfo` for details

##### **quiet**

[bool] pass to `mpfit`. If False, will print out the parameter values for each iteration of the fitter

##### **veryverbose**

[bool] print out a variety of `mpfit` output parameters

##### **debug**

[bool] raise an exception (rather than a warning) if  $\chi^2$  is nan

**n\_modelfunc**(*pars=None*, *debug=False*, *\*\*kwargs*)

Only deals with single-peak functions

**class** pyspeckit.spectrum.models.model.**SpectralModel**(*modelfunc*, *npars*, *shortvarnames=('A',  
'\Delta x', '\sigma')*, *fitunit=None*, *centroid\_par=None*, *fwhm\_func=None*,  
*fwhm\_pars=None*, *integral\_func=None*,  
*use\_lmfit=False*, *guess\_types=('amplitude',  
'center', 'width')*, *\*\*kwargs*)

A wrapper class for a spectra model. Includes internal functions to generate multi-component models, annotations, integrals, and individual components. The declaration can be complex, since you should name individual variables, set limits on them, set the units the fit will be performed in, and set the annotations to be used. Check out some of the hyperfine codes (`hcn`, `n2hp`) for examples.

Spectral Model Initialization

Create a Spectral Model class for data fitting



## Parameters

### **modelfunc**

[function] the model function to be fitted. Should take an X-axis (spectroscopic axis) as an input followed by input parameters. Returns an array with the same shape as the input X-axis

### **npars**

[int] number of parameters required by the model

### **parnames**

[list (optional)] a list or tuple of the parameter names

### **parvalues**

[list (optional)] the initial guesses for the input parameters (defaults to ZEROS)

### **parlimits**

[list (optional)] the upper/lower limits for each variable (defaults to ZEROS)

### **parfixed**

[list (optional)] Can declare any variables to be fixed (defaults to ZEROS)

### **parerror**

[list (optional)] technically an output parameter. Specifying it here will have no effect. (defaults to ZEROS)

### **partied**

[list (optional)] not the past tense of party. Can declare, via text, that some parameters are tied to each other. Defaults to zeros like the others, but it's not clear if that's a sensible default

### **fitunit**

[str (optional)] convert X-axis to these units before passing to model

### **parsteps**

[list (optional)] minimum step size for each parameter (defaults to ZEROS)

### **npeaks**

[list (optional)] default number of peaks to assume when fitting (can be overridden)

### **shortvarnames**

[list (optional)] TeX names of the variables to use when annotating

### **amplitude\_types**

[tuple] A tuple listing the types of the different parameters when guessing. The valid values are 'amplitude', 'width', and 'center'. These are handled by `parse_3par_guesses`, which translate these into input guess lists for the fitter. For a "standard" 3-parameter Gaussian fitter, nothing changes, but for other models that have more than 3 parameters, some translation is needed.

## Returns

A tuple containing (model best-fit parameters, the model, parameter

errors,  $\chi^2$  value)

**`analytic_centroids(centroidpar=None)`**

Return the *analytic* centroids of the model components

### Parameters

#### **centroidpar**

[None or string] The name of the parameter in the fit that represents the centroid *some models have default centroid parameters - these will be used if centroidpar is unspecified*

### Returns

**List of the centroid values (even if there's only 1)**

#### **analytic\_fwhm**(parinfo=None)

Return the FWHM of the model components *if* a fwhm\_func has been defined

Done with incomprehensible list comprehensions instead of nested for loops... readability sacrificed for speed and simplicity. This is unpythonic.

#### **analytic\_integral**(modelpars=None, npeaks=None, npars=None)

Placeholder for analytic integrals; these must be defined for individual models

#### **annotations**(shortvarnames=None, debug=False)

Return a list of TeX-formatted labels

The values and errors are formatted so that only the significant digits are displayed. Rounding is performed using the decimal package.

### Parameters

#### **shortvarnames**

[list] A list of variable names (tex is allowed) to include in the annotations. Defaults to self.shortvarnames

### Examples

```
>>> # Annotate a Gaussian
>>> sp.specfit.annotate(shortvarnames=['A', '\Delta x', '\sigma'])
```

#### **component\_integrals**(xarr, dx=None)

Compute the integrals of each component

#### **components**(xarr, pars, \*\*kwargs)

Return a numpy ndarray of shape [npeaks x modelshape] of the independent components of the fits

#### **computed\_centroid**(xarr=None)

Return the *computed* centroid of the model

### Parameters

#### **xarr**

[None or np.ndarray] The X coordinates of the model over which the centroid should be computed. If unspecified, the centroid will be in pixel units

#### **fitter**(xax, data, err=None, quiet=True, veryverbose=False, debug=False, parinfo=None, \*\*kwargs)

Run the fitter using mpfit.

kwargs will be passed to \_make\_parinfo and mpfit.

**Parameters****xax**

[SpectroscopicAxis] The X-axis of the spectrum

**data**

[ndarray] The data to fit

**err**

[ndarray (optional)] The error on the data. If unspecified, will be uniform unity

**parinfo**[ParinfoList] The guesses, parameter limits, etc. See `pyspeckit.spectrum.parinfo` for details**quiet**

[bool] pass to mpfit. If False, will print out the parameter values for each iteration of the fitter

**veryverbose**

[bool] print out a variety of mpfit output parameters

**debug**[bool] raise an exception (rather than a warning) if  $\chi^2$  is nan**get\_emcee\_ensemblesampler**(*xarr, data, error, nwalkers, \*\*kwargs*)

Get an emcee walker ensemble for the data &amp; model

**Parameters****data**

[np.ndarray]

**error**

[np.ndarray]

**nwalkers**

[int] Number of walkers to use

**Examples**

```

>>> import pyspeckit
>>> x = pyspeckit.units.SpectroscopicAxis(np.linspace(-10,10,50), unit='km/s')
>>> e = np.random.randn(50)
>>> d = np.exp(-np.asarray(x)**2/2.)*5 + e
>>> sp = pyspeckit.Spectrum(data=d, xarr=x, error=np.ones(50)*e.std())
>>> sp.specfit(fittype='gaussian')
>>> nwalkers = sp.specfit.fitter.npars * 2
>>> emcee_ensemble = sp.specfit.fitter.get_emcee_ensemblesampler(sp.xarr, sp.data, sp.error,
↳ nwalkers)
>>> p0 = np.array([sp.specfit.parinfo.values] * nwalkers)
>>> p0 *= np.random.randn(*p0.shape) / 10. + 1.0
>>> pos, logprob, state = emcee_ensemble.run_mcmc(p0, 100)

```

**get\_emcee\_sampler**(*xarr, data, error, \*\*kwargs*)

Get an emcee walker for the data &amp; model

### Parameters

**xarr**  
[pyspeckit.units.SpectroscopicAxis]

**data**  
[np.ndarray]

**error**  
[np.ndarray]

### Examples

```
>>> import pyspeckit
>>> x = pyspeckit.units.SpectroscopicAxis(np.linspace(-10,10,50), unit='km/s')
>>> e = np.random.randn(50)
>>> d = np.exp(-np.asarray(x)**2/2.)*5 + e
>>> sp = pyspeckit.Spectrum(data=d, xarr=x, error=np.ones(50)*e.std())
>>> sp.specfit(fittype='gaussian')
>>> emcee_sampler = sp.specfit.fitter.get_emcee_sampler(sp.xarr, sp.data, sp.error)
>>> p0 = sp.specfit.parinfo
>>> emcee_sampler.run_mcmc(p0,100)
```

**get\_pymc**(xarr, data, error, use\_fitted\_values=False, inf=inf, use\_adaptive=False, return\_dict=False, \*\*kwargs)

Create a pymc MCMC sampler. Defaults to ‘uninformative’ priors

### Parameters

**data**  
[np.ndarray]

**error**  
[np.ndarray]

**use\_fitted\_values**  
[bool] Each parameter with a measured error will have a prior defined by the Normal distribution with sigma = par.error and mean = par.value

**use\_adaptive**  
[bool] Use the Adaptive Metropolis-Hastings sampler?

### Examples

```
>>> x = pyspeckit.units.SpectroscopicAxis(np.linspace(-10,10,50), unit='km/s')
>>> e = np.random.randn(50)
>>> d = np.exp(-np.asarray(x)**2/2.)*5 + e
>>> sp = pyspeckit.Spectrum(data=d, xarr=x, error=np.ones(50)*e.std())
>>> sp.specfit(fittype='gaussian')
>>> MCuninformed = sp.specfit.fitter.get_pymc(sp.xarr, sp.data, sp.error)
>>> MCwithpriors = sp.specfit.fitter.get_pymc(sp.xarr, sp.data, sp.error, use_fitted_
↪ values=True)
>>> MCuninformed.sample(1000)
>>> MCuninformed.stats()['AMPLITUDE0']
>>> # WARNING: This will fail because width cannot be set <0, but it may randomly reach that.
```

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```
>>> # How do you define a likelihood distribution with a lower limit?!
>>> MCwithpriors.sample(1000)
>>> MCwithpriors.stats()['AMPLITUDE0']
```

**integral**(*modelpars*, *dx=None*, *\*\*kwargs*)

Extremely simple integrator: IGNORES *modelpars*; just sums *self.model*

**lmfitfun**(*x*, *y*, *err=None*, *debug=False*)

Wrapper function to compute the fit residuals in an lmfit-friendly format

**lmfitter**(*xax*, *data*, *err=None*, *parinfo=None*, *quiet=True*, *debug=False*, *\*\*kwargs*)

Use lmfit instead of mpfit to do the fitting

#### Parameters

**xax**

[SpectroscopicAxis] The X-axis of the spectrum

**data**

[ndarray] The data to fit

**err**

[ndarray (optional)] The error on the data. If unspecified, will be uniform unity

**parinfo**

[ParinfoList] The guesses, parameter limits, etc. See `pyspeckit.spectrum.parinfo` for details

**quiet**

[bool] If false, print out some messages about the fitting

**logp**(*xarr*, *data*, *error*, *pars=None*)

Return the log probability of the model. If the parameter is out of range, return -inf

**mpfitfun**(*x*, *y*, *err=None*)

Wrapper function to compute the fit residuals in an mpfit-friendly format

**n\_modelfunc**(*pars=None*, *debug=False*, *\*\*kwargs*)

Simple wrapper to deal with N independent peaks for a given spectral model

**parse\_3par\_guesses**(*guesses*)

Try to convert a set of interactive guesses (peak, center, width) into guesses appropriate to the model.

**slope**(*xinp*)

Find the local slope of the model at location *x* (*x* must be in *xax*'s units)

`pyspeckit.spectrum.models.model.parse_offset_guess(gname, gval)`

Utility function for handling guesses. Allows guess types to be specified as 'amplitude\*2' or 'width+3'.

Adds a variable height (background) component to any model

### 3.4.2 Module API



---

## Basic Plotting Guide

---

The plotting tool in pyspeckit is intended to make publication-quality plots straightforward to produce.

For details on the various plotting tools, please see the examples and the [plotter documentation](#).

A few basic examples are shown in the snippet below, with comments describing the various steps:

```
import numpy as np
from astropy import units as u
import pyspeckit

xaxis = np.linspace(-50,150,100.) * u.km/u.s
sigma = 10. * u.km/u.s
center = 50. * u.km/u.s
synth_data = np.exp(-(xaxis-center)**2/(sigma**2 * 2.))

# Add noise
stddev = 0.1
noise = np.random.randn(xaxis.size)*stddev
error = stddev*np.ones_like(synth_data)
data = noise+synth_data

# this will give a "blank header" warning, which is fine
sp = pyspeckit.Spectrum(data=data, error=error, xarr=xaxis,
                        unit=u.erg/u.s/u.cm**2/u.AA)

sp.plotter()
sp.plotter.savefig('basic_plot_example.png')

# Fit with automatic guesses
sp.specfit(fittype='gaussian')
# (this will produce a plot overlay showing the fit curve and values)
sp.plotter.savefig('basic_plot_example_withfit.png')

# Redo the overlay with no annotation
```

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```

# remove both the legend and the model overlay
sp.specfit.clear()
# then re-plot the model without an annotation (legend)
sp.specfit.plot_fit(annotate=False)
sp.plotter.savefig('basic_plot_example_withfit_no_annotation.png')

# overlay another spectrum
# We use the 'synthetic' spectrum with no noise, then shift it by 10 km/s
sp2 = pyspeckit.Spectrum(data=synth_data, error=None, xarr=xaxis+10*u.km/u.s,
                        unit=u.erg/u.s/u.cm**2/u.AA)

# again, remove the overlaid model fit
sp.specfit.clear()

# to overplot, you need to tell the plotter which matplotlib axis to use and
# tell it not to clear the plot first
sp2.plotter(axis=sp.plotter.axis,
            clear=False,
            color='g')

# sp2.plotter and sp.plotter can both be used here (they refer to the same axis
# and figure now)
sp.plotter.savefig('basic_plot_example_with_second_spectrum_overlaid_in_green.png')

# the plot window will follow the last plotted spectrum's limits by default;
# that can be overridden with the xmin/xmax keywords
sp2.plotter(axis=sp.plotter.axis,
            xmin=-100, xmax=200,
            ymin=-0.5, ymax=1.5,
            clear=False,
            color='g')
sp.plotter.savefig('basic_plot_example_with_second_spectrum_overlaid_in_green_wider_limits.png')

# you can also offset the spectra and set different
# this time, we need to clear the axis first, then do a fresh overlay

# fresh plot
sp.plotter(clear=True)

# overlay, shifted down by 0.2 in y and with a wider linewidth
sp2.plotter(axis=sp.plotter.axis,
            offset=-0.2,
            clear=False,
            color='r',
            linewidth=2,
            alpha=0.5,
            )
# you can also modify the axis properties directly
sp.plotter.axis.set_ylim(-0.25, 1.1)
sp2.plotter.savefig('basic_plot_example_with_second_spectrum_offset_overlaid_in_red.png')

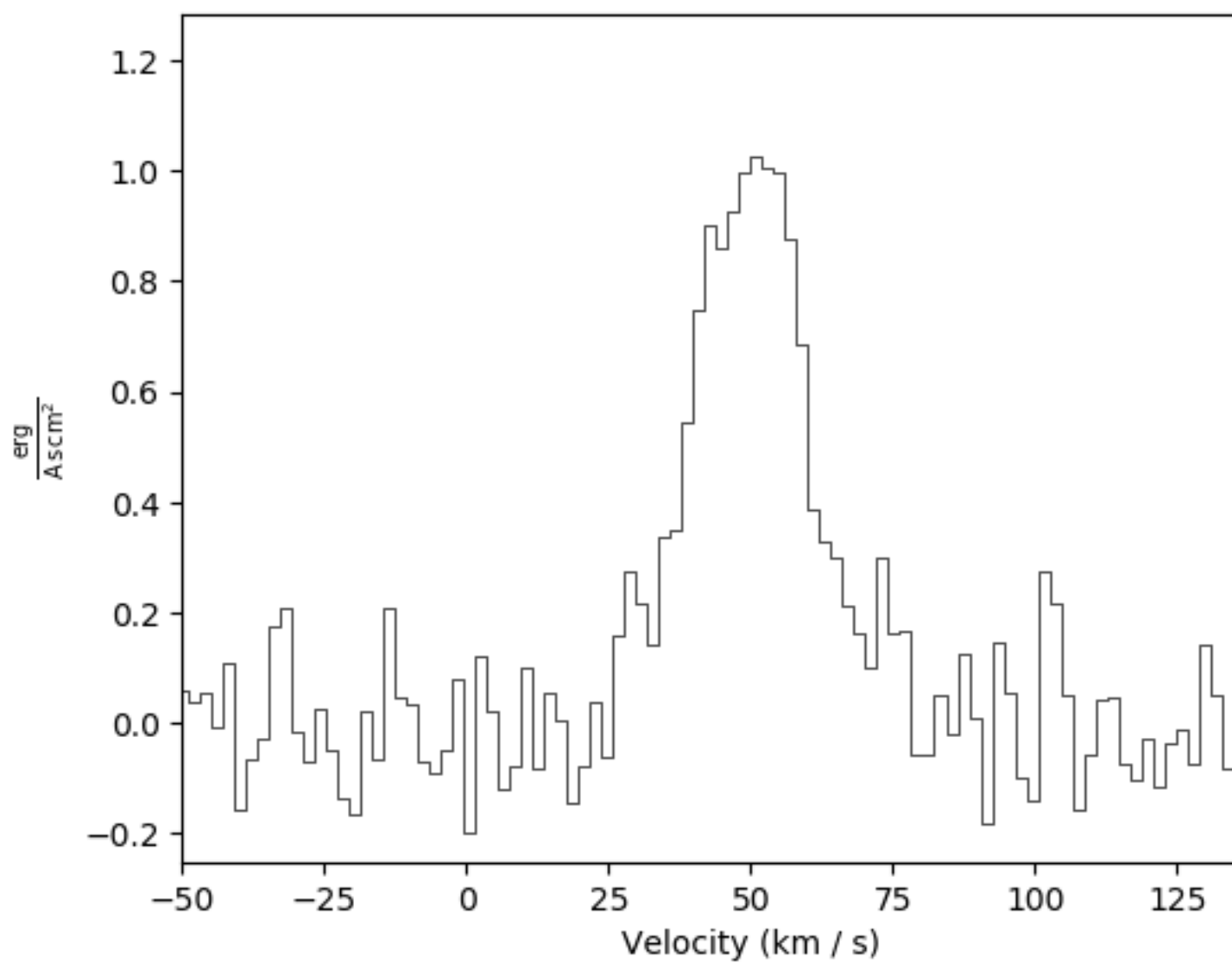
```

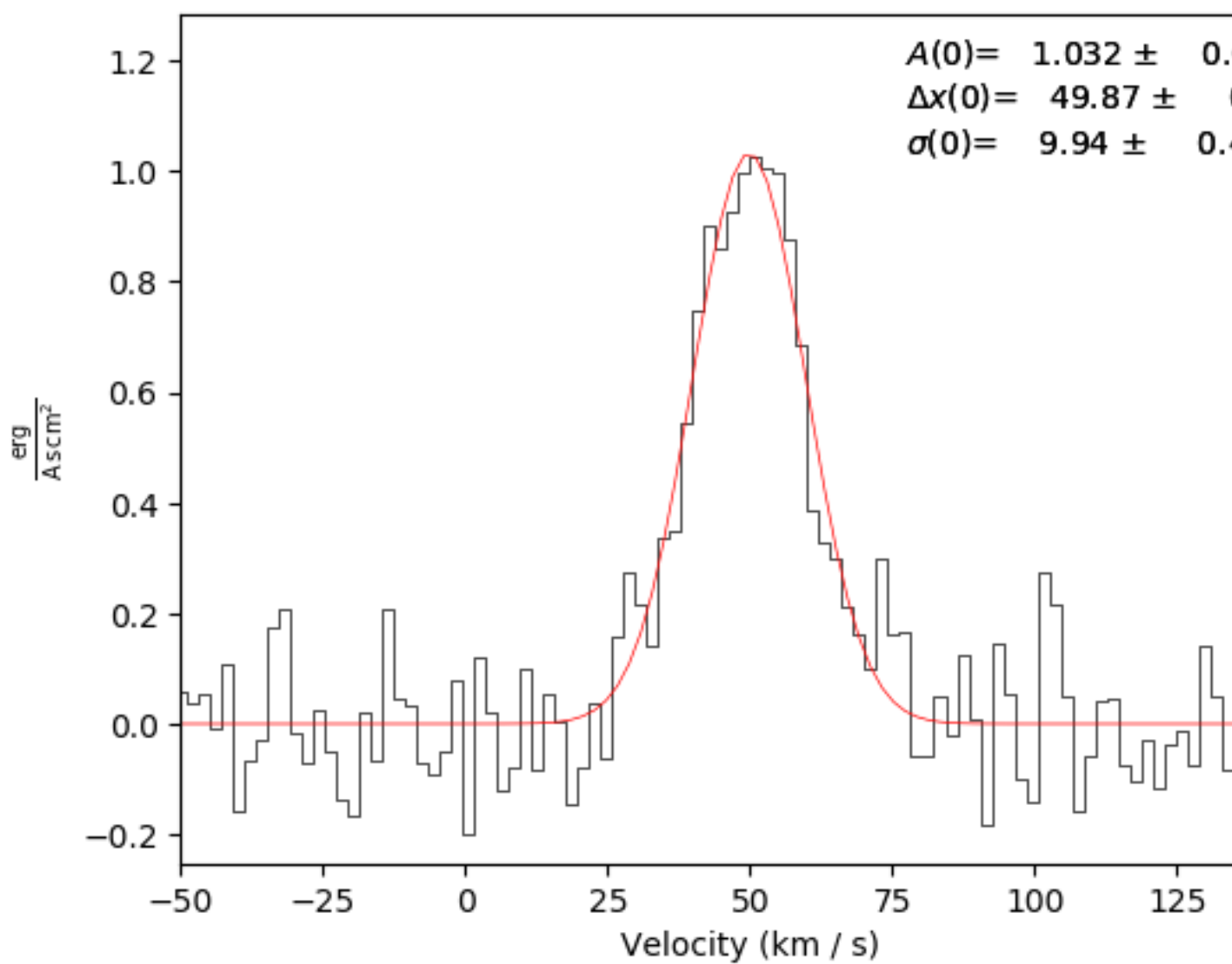
Basic plot example:

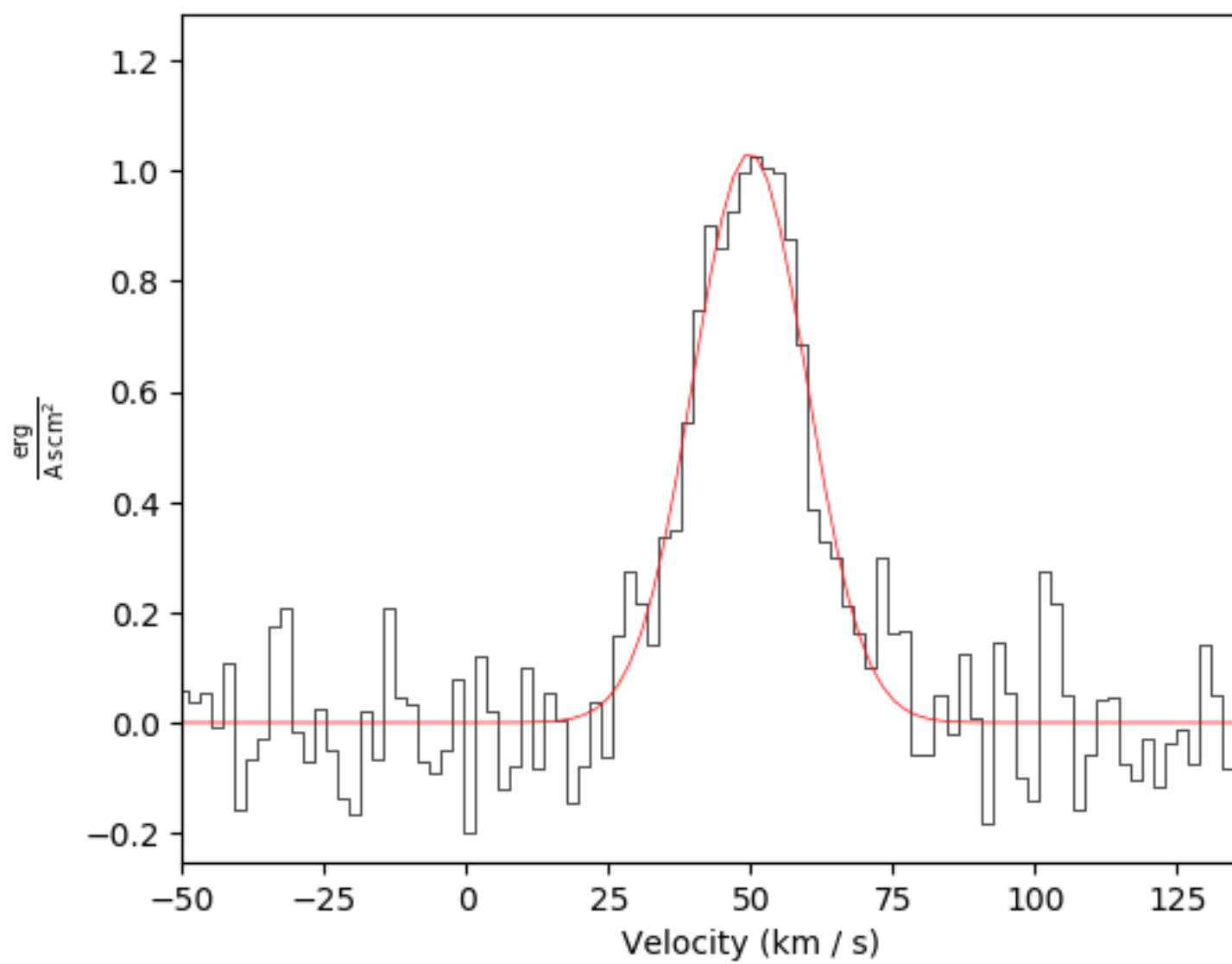
Basic plot example with a fit and an annotation (annotation is on by default):

Basic plot example with a fit, but with no annotation:

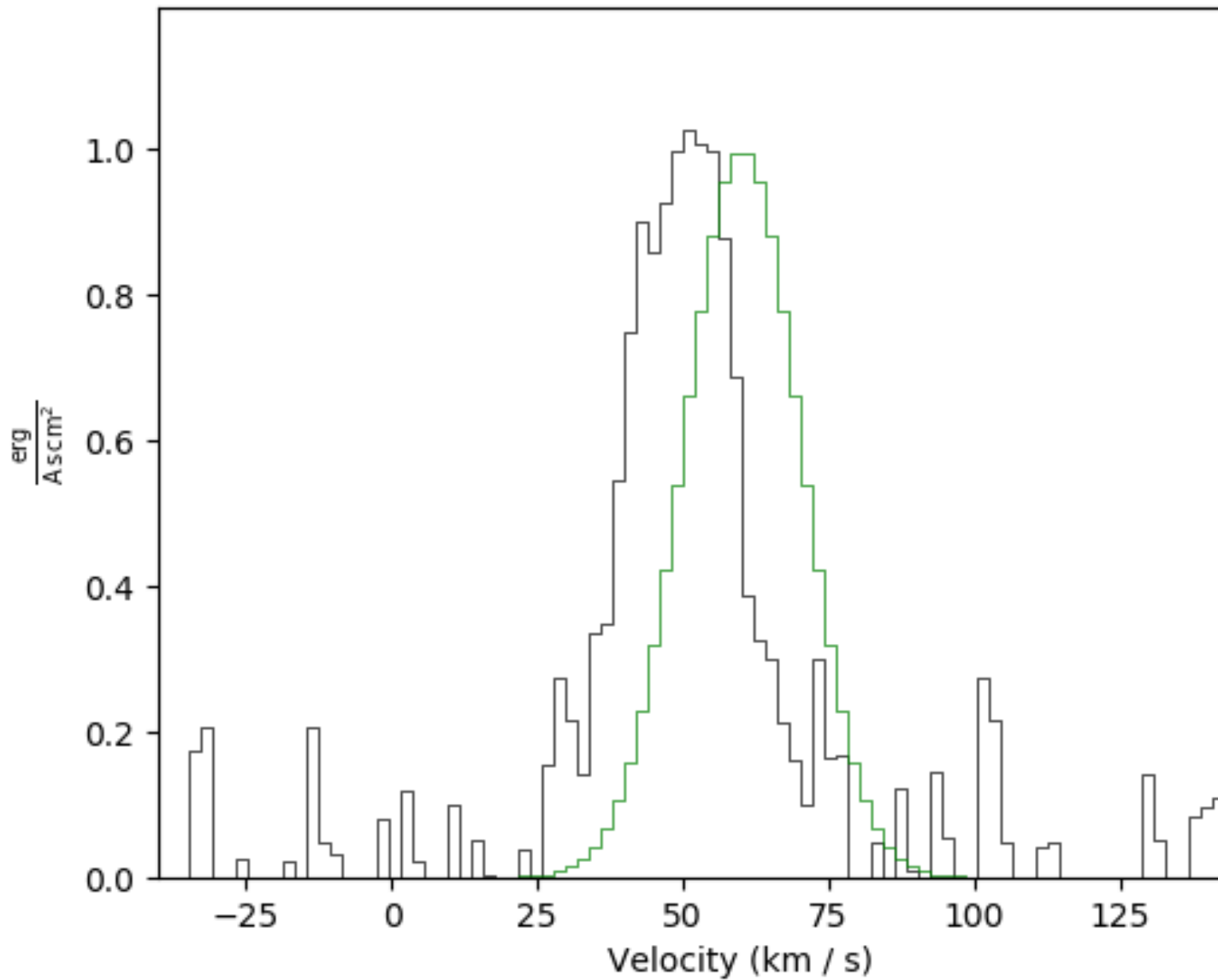








Basic plot example with a second spectrum overlaid in green:



Basic plot example with a second spectrum overlaid in green plus adjusted limits:

Basic plot example with a second spectrum offset and overlaid in red, again with adjusted limits:

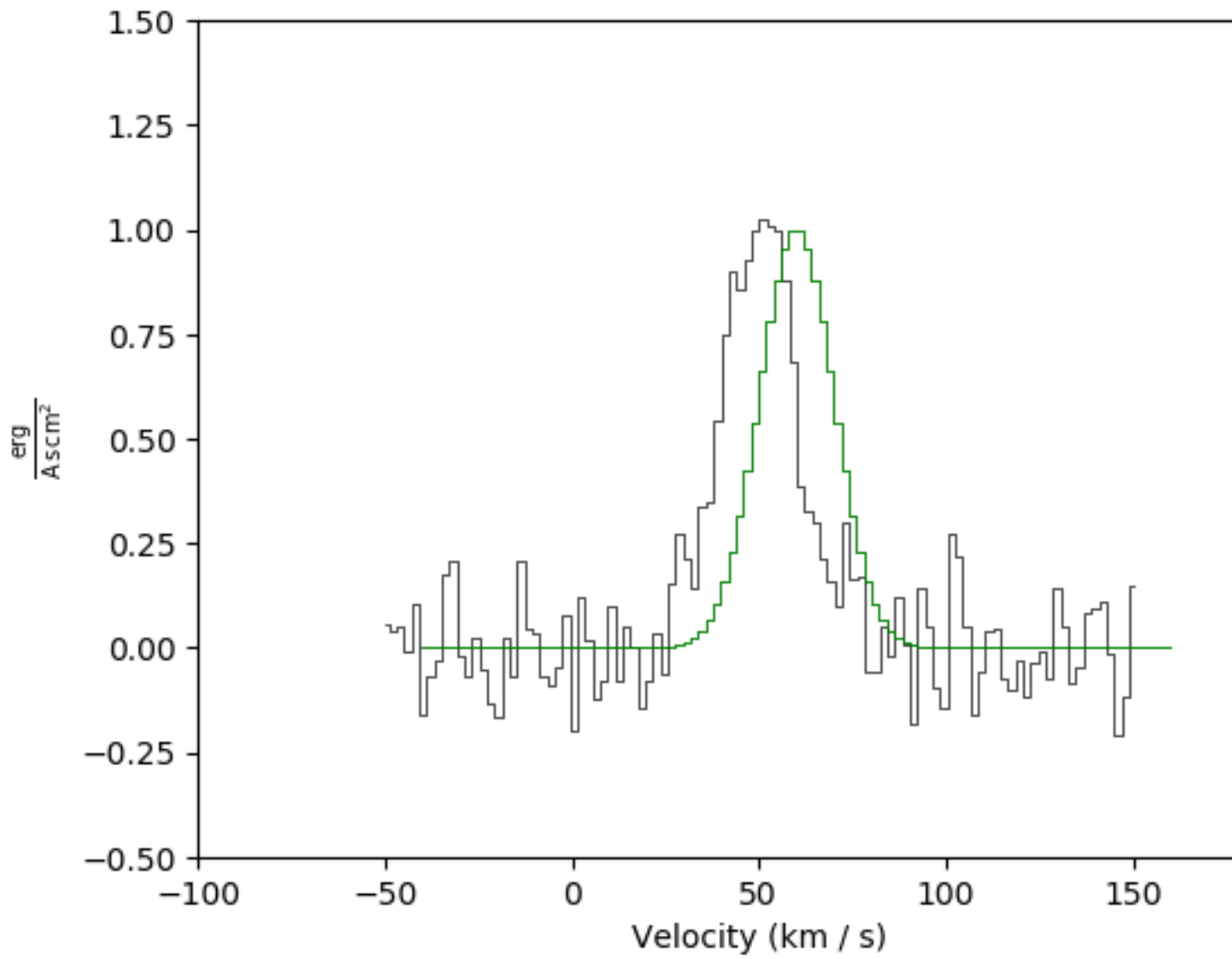
## 4.1 API Documentation for Plotting

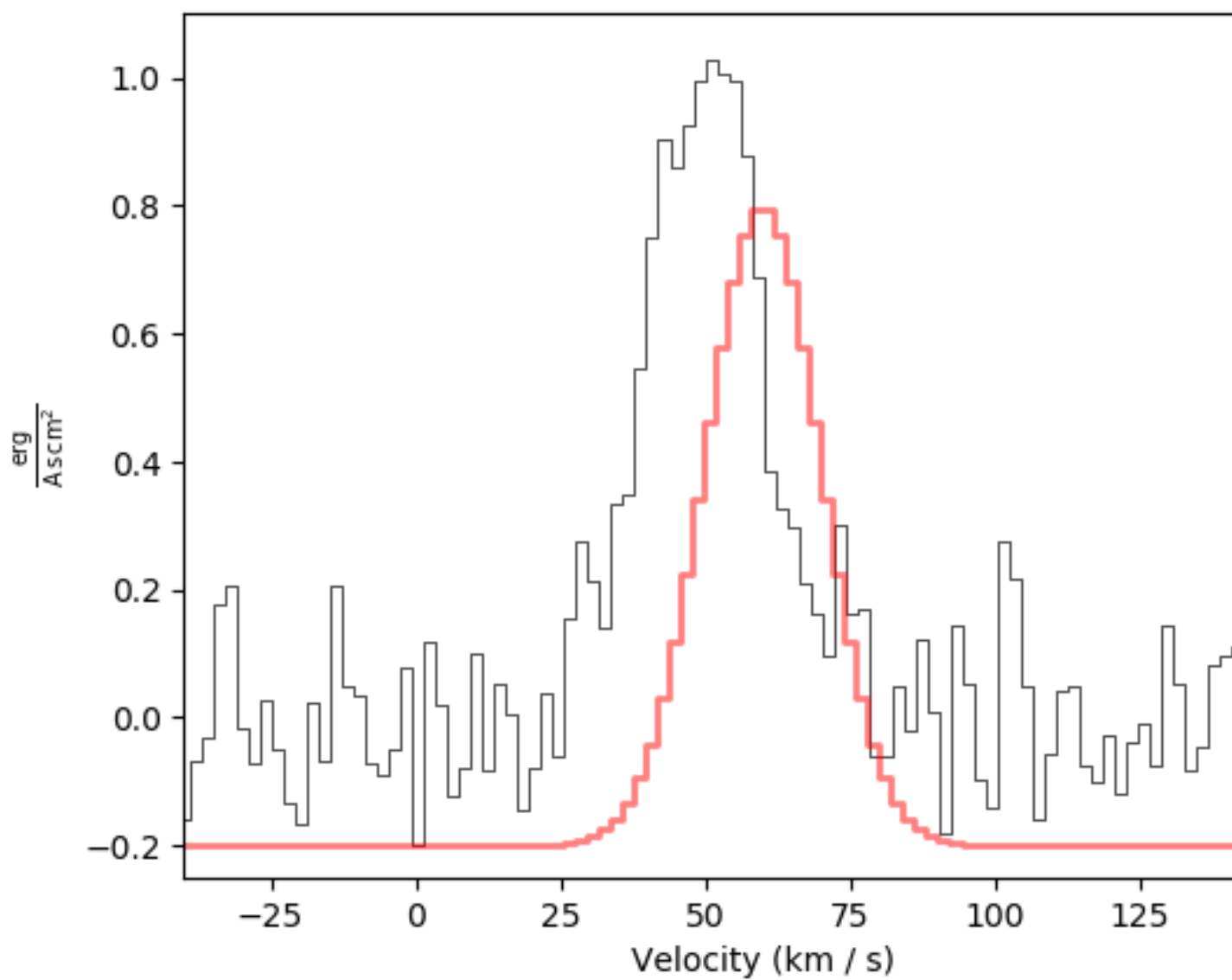
We include the API documentation for the generic model and fitter wrappers here.

```
class pyspeckit.spectrum.plotters.Plotter(Spectrum, autorefresh=True, title="", xlabel=None,  
                                           silent=True, plotscale=1.0, **kwargs)
```

Class to plot a spectrum

```
activate_interactive_baseline_fitter(**kwargs)  
    Attempt to activate the interactive baseline fitter
```





**activate\_interactive\_fitter()**

Attempt to activate the interactive fitter

**connect()**

Connect to the matplotlib key-parsing interactivity

**copy**(*parent=None*)

Create a copy of the plotter with blank (uninitialized) axis & figure

**[ parent ]**

A spectroscopic axis instance that is the parent of the specfit instance. This needs to be specified at some point, but defaults to None to prevent overwriting a previous plot.

**disconnect()**

Disconnect the matplotlib interactivity of this pyspeckit plotter.

**label**(*title=None, xlabel=None, ylabel=None, verbose\_label=False, \*\*kwargs*)

Label the plot, with an attempt to parse standard units into nice latex labels

#### Parameters

**title**

[str]

**xlabel**

[str]

**ylabel**

[str]

**verbose\_label: bool**

**line\_ids**(*line\_names, line\_xvals, xval\_units=None, auto\_yloc=True, velocity\_offset=None, velocity\_convention='radio', auto\_yloc\_fraction=0.9, \*\*kwargs*)

Add line ID labels to a plot using lineid\_plot <http://oneau.wordpress.com/2011/10/01/line-id-plot/>  
[https://github.com/phn/lineid\\_plot](https://github.com/phn/lineid_plot) [http://packages.python.org/lineid\\_plot/](http://packages.python.org/lineid_plot/)

#### Parameters

**line\_names**

[list] A list of strings to label the specified x-axis values

**line\_xvals**

[list] List of x-axis values (e.g., wavelengths) at which to label the lines. Can be a list of quantities.

**xval\_units**

[string] The unit of the line\_xvals if they are not given as quantities

**velocity\_offset**

[quantity] A velocity offset to apply to the inputs if they are in frequency or wavelength units

**velocity\_convention**

['radio' or 'optical' or 'doppler'] Used if the velocity offset is given

**auto\_yloc**

[bool] If set, overrides box\_loc and arrow\_tip (the vertical position of the lineid labels) in kwargs to be auto\_yloc\_fraction of the plot range

**auto\_yloc\_fraction: float in range [0,1]**

The fraction of the plot (vertically) at which to place labels

## Examples

```
>>> import numpy as np
>>> import pyspeckit
>>> sp = pyspeckit.Spectrum(
    xarr=pyspeckit.units.SpectroscopicAxis(np.linspace(-50,50,101),
        unit='km/s', refX=6562.8, refX_unit='angstrom'),
    data=np.random.randn(101), error=np.ones(101))
>>> sp.plotter()
>>> sp.plotter.line_ids(['H$\alpha$'], [6562.8], xval_units='angstrom')
```

**line\_ids\_from\_measurements**(*auto\_yloc=True, auto\_yloc\_fraction=0.9, \*\*kwargs*)

Add line ID labels to a plot using `lineid_plot` <http://oneau.wordpress.com/2011/10/01/line-id-plot/>  
[https://github.com/phn/lineid\\_plot](https://github.com/phn/lineid_plot) [http://packages.python.org/lineid\\_plot/](http://packages.python.org/lineid_plot/)

## Parameters

**auto\_yloc**

[bool] If set, overrides `box_loc` and `arrow_tip` (the vertical position of the lineid labels) in `kwargs` to be `auto_yloc_fraction` of the plot range

**auto\_yloc\_fraction: float in range [0,1]**

The fraction of the plot (vertically) at which to place labels

## Examples

```
>>> import numpy as np
>>> import pyspeckit
>>> sp = pyspeckit.Spectrum(
    xarr=pyspeckit.units.SpectroscopicAxis(np.linspace(-50,50,101),
        units='km/s', refX=6562.8, refX_unit='angstroms'),
    data=np.random.randn(101), error=np.ones(101))
>>> sp.plotter()
>>> sp.specfit(multifit=None, fittype='gaussian', guesses=[1,0,1]) # fitting noise...
>>> sp.measure()
>>> sp.plotter.line_ids_from_measurements()
```

**parse\_keys**(*event*)

Parse key commands entered from the keyboard

**plot**(*offset=0.0, xoffset=0.0, color='k', linestyle='steps-mid', linewidth=0.5, errstyle=None, erralpha=0.2, errcolor=None, silent=None, reset=True, refresh=True, use\_window\_limits=None, use\_offset=False, \*\*kwargs*)  
Plot the spectrum!

Tries to automatically find a reasonable plotting range if one is not set.

## Parameters

**offset**

[float] vertical offset to add to the spectrum before plotting. Useful if you want to overlay multiple spectra on a single plot



**xoffset: float**

An x-axis shift. I don't know why you'd want this...

**color**

[str] default to plotting spectrum in black

**linestyle**

['steps-mid' or str] 'steps-mid' for histogram-style plotting. See matplotlib's plot for more information

**linewidth**

[float] Line width in pixels. Narrow lines are helpful when histo-plotting

**errstyle**

['fill', 'bars', or None] can be "fill", which draws partially transparent boxes around the data to show the error region, or "bars" which draws standard errorbars. None will display no errorbars

**useOffset**

[bool] Use offset-style X/Y coordinates (e.g., 1 + 1.483e10)? Defaults to False because these are usually quite annoying.

**xmin/xmax/ymin/ymax**

[float] override defaults for plot range. Once set, these parameters are sticky (i.e., replotting will use the same ranges). Passed to [reset\\_limits](#)

**reset\_[xy]limits**

[bool] Reset the limits to "sensible defaults". Passed to [reset\\_limits](#)

**ypeakscale**

[float] Scale up the Y maximum value. Useful to keep the annotations away from the data. Passed to [reset\\_limits](#)

**reset**

[bool] Reset the x/y axis limits? If set, [reset\\_limits](#) will be called.

**reset\_limits**(xmin=None, xmax=None, ymin=None, ymax=None, reset\_xlimits=True, reset\_ylimits=True, ypeakscale=1.2, silent=None, use\_window\_limits=False, \*\*kwargs)  
Automatically or manually reset the plot limits

**savefig**(fname, bbox\_inches='tight', \*\*kwargs)  
simple wrapper of matplotlib's savefig.

**set\_limits\_from\_visible\_window**(debug=False)

Hopefully self-descriptive: set the x and y limits from the currently visible window (use this if you use the pan/zoom tools or manually change the limits)

pyspeckit.spectrum.plotters.**parse\_norm**(norm)

Expected format: norm = 10E15

pyspeckit.spectrum.plotters.**steppify**(arr, isX=False)

*support function* Converts an array to double-length for step plotting



## 5.1 Baseline Fitting

There are a number of cool features in baselining that aren't well-described below, partly due to Sphinx errors as of 12/22/2011.

`exclude` and `include` allow you to specify which parts of the spectrum to use for baseline fitting. Enter values as pairs of coordinates.

`Excludefit` makes use of an existing fit and excludes all points with signal above a (very low) threshold when fitting the baseline. Going back and forth between `baseline(excludefit=True)` and `specfit()` is a nice way to iteratively measure the baseline & emission/absorption line components.

### 5.1.1 API

**class** `pyspeckit.spectrum.baseline.Baseline(Spectrum)`

Class to measure and subtract baselines from spectra.

While the term 'baseline' is generally used in the radio to refer to broad-band features in a spectrum not necessarily associated with a source, in this package it refers to general continuum fitting. In principle, there's no reason to separate 'continuum' and 'spectral feature' fitting into different categories (both require some model, data, and optional weights when fitting). In practice, however, 'continuum' is frequently something to be removed and ignored, while spectral features are the desired measurable quantity. In order to accurately measure spectral features, it is necessary to allow baselines of varying complexity.

The `Baseline` class has both interactive and command-based data selection features. It can be used to fit both polynomial and power-law continua. Blackbody fitting is not yet implemented [12/21/2011]. Baseline fitting is a necessary prerequisite for Equivalent Width measurement.

As you may observe in the comments on this code, this has been one of the buggiest and least adequately tested components of `pyspeckit`. Bug reports are welcome. (as of 1/15/2012, a major change has probably fixed most of the bugs, and the code base is much simpler)

**\_\_call\_\_**(\*args, \*\*kwargs)

Fit and remove a polynomial from the spectrum. It will be saved in the variable “self.basespec” and the fit parameters will be saved in “self.order”

### Parameters

**order: int**

Order of the polynomial to fit

**excludefit: bool**

If there is a spectroscopic line fit, you can automatically exclude the region with signal above some tolerance set by `exclusionlevel` (it works for absorption lines by using the absolute value of the signal)

**exclusionlevel: float**

The minimum value of the spectroscopic fit to exclude when fitting the baseline

**save: bool**

Write the baseline fit coefficients into the spectrum’s header in the keywords `BLCOEFnn`

**interactive: bool**

Specify the include/exclude regions through the interactive plot window

**fit\_original: bool**

Fit the original spectrum instead of the baseline-subtracted spectrum. If disabled, will overwrite the original data with the baseline-subtracted version.

**Warning:** If this is set False, behavior of `unsubtract` may be unexpected

**fit\_plotted\_area: bool**

Will respect user-specified zoom (using the pan/zoom buttons) unless `xmin/xmax` have been set manually

**reset\_selection: bool**

Reset the selected region to those specified by this command only (will override previous `xmin/xmax` settings)

**select\_region: bool**

Run the region selection procedure? If false, will leave ‘`includemask`’ untouched

**baseline\_fit\_color: color name (string)**

[plot parameter] Color to plot the baseline

**clear\_all\_connections: bool**

[plot parameter] Disable any previous interactive sessions

**highlight\_fitregion: bool**

[plot parameter] Highlight the selected region for baseline fitting (default green)

**\_\_init\_\_**(*Spectrum*)

Declare interactive variables.

Must have a parent `Spectrum` class

**Must declare `button2action` and `button3action`**

**\_\_module\_\_** = 'pyspeckit.spectrum.baseline'

**annotate**(*loc*='upper left', *fontsize*=10)

**button2action**(*event*=None, *debug*=False, *subtract*=True, *powerlaw*=None, *fit\_original*=False, *spline*=False, *spline\_sampling*=None, *spline\_downsampler*=<function median>, *baseline\_fit\_color*='orange', \*\*kwargs)

Do the baseline fitting and save and plot the results.

Note that powerlaw fitting will only consider positive data.

**button3action**(\*args, \*\*kwargs)

Wrapper - same as button2action, but with subtract=False

**clearlegend**()

**copy**(*parent*=None)

Create a copy of the baseline fit

[ **parent** ]

A spectroscopic axis instance that is the parent of the specfit instance. This needs to be specified at some point, but defaults to None to prevent overwriting a previous plot.

**crop**(*x1pix*, *x2pix*)

When spectrum.crop is called, this must be too

**downsample**(*factor*)

**fit**(*powerlaw*=None, *order*=None, *includemask*=None, *spline*=False, *spline\_sampling*=10, *spline\_downsampler*=<function median>, *xarr\_fit\_unit*='pixels', \*\*kwargs)

Run the fit and set self.basespec

**get\_model**(*xarr*=None, *baselinepars*=None)

**plot\_baseline**(*annotate*=True, *baseline\_fit\_color*='orange', *use\_window\_limits*=None, *linewidth*=1, *alpha*=0.75, *plotkwargs*={}, \*\*kwargs)

Overplot the baseline fit

### Parameters

#### **annotate**

[bool] Display the fit parameters for the best-fit baseline on the top-left of the plot

#### **baseline\_fit\_color**

[matplotlib color] What color to use for overplotting the line (default is slightly transparent orange)

#### **use\_window\_limits**

[None or bool] Keep the current window or expand the plot limits? If left as None, will use self.use\_window\_limits

### Other Parameters

#### **linewidth**

[number]

#### **alpha**

[float [0-1]]

**plotkwargs**

[dict] Are passed to matplotlib's plot function

**savefit()****set\_basespec\_frompars**(*baselinepars=None, xarr\_fit\_unit=None*)

Set the baseline spectrum based on the fitted parameters

**Parameters****baselinepars**

[list] Optional list of fit parameters, e.g. a list of polynomial coefficients

**xarr\_fit\_unit**

[None or 'pixels' or 'native' or unit] The units that were used in the baseline fit

**set\_spectofit**(*fit\_original=True, fit\_residuals=False*)

Reset the spectrum-to-fit from the data

**unsubtract**(*replot=True, preserve\_limits=True*)

Restore the spectrum to "pristine" state (un-subtract the baseline)

**replot** [ True ]

Re-plot the spectrum? (only happens if unsubtraction proceeds, i.e. if there was a baseline to unsubtract)

**preserve\_limits** [ True ]

Preserve the current x,y limits

## 5.2 Model Fitting

**class** pyspeckit.spectrum.fitters.**Specfit**(*Spectrum, Registry=None*)

Bases: pyspeckit.spectrum.interactive.Interactive

**EQW**(*plot=False, plotcolor='g', fitted=True, continuum=None, components=False, annotate=False, alpha=0.5, loc='lower left', xmin=None, xmax=None, xunits=None, continuum\_as\_baseline=False, xunit='pixel', midpt\_location='plot-center'*)

Returns the equivalent width (integral of "baseline" or "continuum" minus the spectrum) over the selected range (the selected range defaults to self.xmin:self.xmax, so it may include multiple lines!)

**Parameters****plot**

[bool] Plots a box indicating the EQW if plot==True (i.e., it will have a width equal to the equivalent width, and a height equal to the measured continuum)

**fitted**

[bool] Use the fitted model? If false, uses the data

**continuum**

[None or float] Can specify a fixed continuum with this keyword, otherwise will use the fitted baseline. **WARNING:** continuum=0 will still "work", but will give numerically invalid results. Similarly, a negative continuum will work, but will yield results with questionable physical meaning.

**continuum\_as\_baseline**

[bool] Replace the baseline with the specified continuum when computing the absorption depth of the line

**components**

[bool] If your fit is multi-component, will attempt to acquire centroids for each component and print out individual EQWs

**xmin**

[float]

**xmax**

[float] The range over which to compute the EQW

**xunit**

[str] The units of xmin/xmax

**midpt\_location**

['fitted', 'plot-center'] If 'plot' is set, this determines where the EQW will be drawn. It can be the fitted centroid or the plot-center, i.e.  $(x_{\min} + x_{\max})/2$

**Returns**

**Equivalent Width, or widths if components=True**

**add\_sliders**(*parlimitdict=None, \*\*kwargs*)

Add a Sliders window in a new figure appropriately titled

**Parameters****parlimitdict: dict**

Each parameter needs to have displayed limits; these are set in min-max pairs. If this is left empty, the widget will try to guess at reasonable limits, but the guessing is not very sophisticated yet.

**.. todo:: Add a button in the navbar that makes this window pop up**

<http://stackoverflow.com/questions/4740988/add-new-navigate-modes-in-matplotlib>

**annotate**(*loc='upper right', labelspacing=0.25, markerscale=0.01, borderpad=0.1, handlelength=0.1, handletextpad=0.1, fontsize=10, frameon=False, chi2=None, optimal\_chi2\_kwargs={}, \*\*kwargs*)

Add a legend to the plot showing the fitted parameters

`_clearlegend()` will remove the legend

`chi2`: {True or 'reduced' or 'optimal' or 'allthree'}

`kwargs` passed to legend

**button3action**(*event, debug=False, nwidths=1*)

Disconnect the interactiveness Perform the fit (or die trying) Hide the guesses

**clear**(*legend=True, components=True*)

Remove the fitted model from the plot

Also removes the legend by default

**clear\_all\_connections**(*debug=False*)

Prevent overlapping interactive sessions

**clear\_highlights**()

Hide and remove “highlight” colors from the plot indicating the selected region

**copy**(*parent=None, registry=None*)

Create a copy of the spectral fit - includes copies of the `_full_model`, the registry, the fitter, `parinfo`, `modelpars`, `modelerrs`, `model`, `npeaks`

#### Parameters

##### **parent**

[`pyspeckit.classes.Spectrum`] A `Spectrum` instance that is the parent of the `specfit` instance. This needs to be specified at some point, but defaults to `None` to prevent overwriting a previous plot.

**crop**(*x1pix, x2pix*)

When `spectrum.crop` is called, this must be too

**dof**

degrees of freedom in fit

**downsample**(*factor*)

Downsample the model spectrum (and the `specfit` spectra) This should only be done when `Spectrum.smooth` is called

**event\_manager**(*event, force\_over\_toolbar=False, debug=False*)

Decide what to do given input (click, keypress, etc.)

**firstclick\_guess**()

Initialize `self.guesses`

**fitter**

**fullsizemodel**()

If the model was fit to a sub-region of the spectrum, expand it (with zeros wherever the model was not defined) to fill the spectrum.

## Examples

```
>>> noise = np.random.randn(100)
>>> xarr = np.linspace(-50,50,100)
>>> signal = np.exp(-(xarr-5)**2/(2*3.**2))
>>> sp = pyspeckit.Spectrum(data=noise + signal, xarr=xarr, xarrkwargs={'units':'km/s'})
>>> sp.specfit(xmin=-25,xmax=25)
>>> sp.specfit.model.shape
(48,)
>>> sp.specfit.fullsizemodel()
>>> sp.specfit.model.shape
(100,)
```

**get\_components**(*\*\*kwargs*)

If a model has been fitted, return the components of the model

#### Parameters



kwargs are passed to `self.fitter.components`

**get\_emcee**(*nwalkers=None*, *\*\*kwargs*)

Get an emcee walker ensemble for the data & model using the current model type

#### Parameters

**data**

[np.ndarray]

**error**

[np.ndarray]

**nwalkers**

[int] Number of walkers to use. Defaults to  $2 * \text{self.fitters.npars}$

#### Examples

```
>>> import pyspeckit
>>> x = pyspeckit.units.SpectroscopicAxis(np.linspace(-10,10,50), unit='km/s')
>>> e = np.random.randn(50)
>>> d = np.exp(-np.asarray(x)**2/2.)*5 + e
>>> sp = pyspeckit.Spectrum(data=d, xarr=x, error=np.ones(50)*e.std())
>>> sp.specfit(fittype='gaussian')
>>> emcee_ensemble = sp.specfit.get_emcee()
>>> p0 = emcee_ensemble.p0 * (np.random.randn(*emcee_ensemble.p0.shape) / 10. + 1.0)
>>> pos, logprob, state = emcee_ensemble.run_mcmc(p0, 100)
```

**get\_full\_model**(*debug=False*, *\*\*kwargs*)

compute the model over the full axis

**get\_model**(*xarr*, *pars=None*, *debug=False*, *add\_baseline=None*)

Compute the model over a given axis

**get\_model\_frompars**(*xarr*, *pars*, *debug=False*, *add\_baseline=None*)

Compute the model over a given axis

**get\_model\_xlimits**(*threshold='auto'*, *peak\_fraction=0.01*, *add\_baseline=False*, *unit='pixels'*, *units=None*)

Return the x positions of the first and last points at which the model is above some threshold

#### Parameters

**threshold**

['auto' or 'error' or float] If 'auto', the threshold will be set to  $\text{peak\_fraction} * \text{the peak model value}$ . If 'error', uses the error spectrum as the threshold

**peak\_fraction**

[float] ignored unless threshold == 'auto'

**add\_baseline**

[bool] Include the baseline when computing whether the model is above the threshold? default FALSE. Passed to `get_full_model`.

**units**

[str] A valid unit type, e.g. 'pixels' or 'angstroms'

**get\_pymc**(\*\*kwargs)

Create a pymc MCMC sampler from the current fitter. Defaults to ‘uninformative’ priors

kwargs are passed to the fitter’s get\_pymc method, with parameters defined below.

#### Parameters

**data**

[np.ndarray]

**error**

[np.ndarray]

**use\_fitted\_values**

[bool] Each parameter with a measured error will have a prior defined by the Normal distribution with  $\sigma = \text{par.error}$  and  $\mu = \text{par.value}$

#### Examples

```
>>> x = pyspeckit.units.SpectroscopicAxis(np.linspace(-10,10,50), unit='km/s')
>>> e = np.random.randn(50)
>>> d = np.exp(-np.asarray(x)**2/2.)*5 + e
>>> sp = pyspeckit.Spectrum(data=d, xarr=x, error=np.ones(50)*e.std())
>>> sp.specfit(fittype='gaussian')
>>> MCuninformed = sp.specfit.get_pymc()
>>> MCwithpriors = sp.specfit.get_pymc(use_fitted_values=True)
>>> MCuninformed.sample(1000)
>>> MCuninformed.stats()['AMPLITUDE0']
>>> # WARNING: This will fail because width cannot be set <0, but it may randomly reach that.
↪...
>>> # How do you define a likelihood distribution with a lower limit?!
>>> MCwithpriors.sample(1000)
>>> MCwithpriors.stats()['AMPLITUDE0']
```

**guesspeakwidth**(event, debug=False, nwidths=1, \*\*kwargs)

Interactively guess the peak height and width from user input

Width is assumed to be half-width-half-max

**highlight\_fitregion**(drawstyle='steps-mid', color=(0, 0.8, 0, 0.5), linewidth=2, alpha=0.5, clear\_highlights=True, \*\*kwargs)

Re-highlight the fitted region

kwargs are passed to matplotlib.plot

**history\_fitpars**()

**integral**(analytic=False, direct=False, threshold='auto', integration\_limits=None, integration\_limit\_units='pixels', return\_error=False, \*\*kwargs)

Return the integral of the fitted spectrum

#### Parameters

**analytic**

[bool] Return the analytic integral of the fitted function? .. WARNING:: This approach is only implemented for some models .. todo:: Implement error propagation for this approach

**direct**

[bool] Return the integral of the *spectrum* (as opposed to the *fit*) over a range defined by the *integration\_limits* if specified or *threshold* otherwise

**threshold**

['auto' or 'error' or float] Determines what data to be included in the integral based off of where the model is greater than this number. If 'auto', the threshold will be set to  $\text{peak\_fraction} * \text{the peak model value}$ . If 'error', uses the error spectrum as the threshold. See `self.get_model_xlimits` for details

**integration\_limits**

[None or 2-tuple] Manually specify the limits in *integration\_limit\_units* units

**return\_error**

[bool] Return the error on the integral if set. The error computed by  $\sigma = \sqrt{\sum(\sigma_i^2)} * dx$

**kwargs :**

passed to `self.fitter.integral` if not(*direct*)

**Returns**

**np.scalar or np.ndarray with the integral or integral & error**

**mask**

Mask: True means "exclude"

**mask\_sliced**

Sliced (subset) Mask: True means "exclude"

**measure\_approximate\_fwhm**(*threshold='error', emission=True, interpolate\_factor=1, plot=False, grow\_threshold=2, \*\*kwargs*)

Measure the FWHM of a fitted line

This procedure is designed for multi-component *blended* lines; if the true FWHM is known (i.e., the line is well-represented by a single gauss/voigt/lorentz profile), use that instead. Do not use this for multiple independently peaked profiles.

This MUST be run AFTER a fit has been performed!

**Parameters****threshold**

['error' | float] The threshold above which the spectrum will be interpreted as part of the line. This threshold is applied to the *model*. If it is 'noise', `self.error` will be used.

**emission**

[bool] Is the line absorption or emission?

**interpolate\_factor**

[integer] Magnification factor for determining sub-pixel FWHM. If used, "zooms-in" by using linear interpolation within the line region

**plot**

[bool] Overplot a line at the FWHM indicating the FWHM. *kwargs* are passed to `matplotlib.plot`

**grow\_threshold**

[int] Minimum number of valid points. If the total # of points above the threshold is  $\leq$  to this number, it will be grown by 1 pixel on each side

### Returns

The approximated FWHM, if it can be computed

If there are  $\leq 2$  valid pixels, a fwhm cannot be computed

**model\_mask**(\*\*kwargs)

Get a mask (boolean array) of the region where the fitted model is significant

### Parameters

#### threshold

[‘auto’ or ‘error’ or float] The threshold to compare the model values to for selecting the mask region.

- auto: uses peak\_fraction times the model peak
- error: use the spectrum error
- float: any floating point number as an absolute threshold

#### peak\_fraction

[float] Parameter used if threshold==‘auto’ to determine fraction of model peak to set threshold at

#### add\_baseline

[bool] Add the fitted baseline to the model before comparing to threshold?

### Returns

#### mask

[ndarray] A boolean mask array with the same size as the spectrum, set to True where the fitted model has values above a specified threshold

**moments**(fittype=None, \*\*kwargs)

Return the moments

see the moments module

### Parameters

#### fittype

[None or str] The registered fit type to use for moment computation

**multifit**(fittype=None, renormalize=‘auto’, annotate=None, show\_components=None, verbose=True, color=None, guesses=None, parinfo=None, reset\_fitspec=True, use\_window\_limits=None, use\_lmfit=False, plot=True, \*\*kwargs)

Fit multiple gaussians (or other profiles)

### Parameters

#### fittype

[str] What function will be fit? fittype must have been Registryed in the peakbgfitters dict. Uses default (‘gaussian’) if not specified

**renormalize**

[‘auto’ or bool] if ‘auto’ or True, will attempt to rescale small data (<1e-9) to be closer to 1 (scales by the median) so that the fit converges better

**parinfo**

[parinfo structure] Guess structure; supercedes guesses

**guesses**

[list or ‘moments’] Either a list of guesses matching the number of parameters \* the number of peaks for the model, or ‘moments’ to fit a single spectrum with the moments as guesses

**optimal\_chi2**(*reduced=True, threshold=‘error’, \*\*kwargs*)

Compute an “optimal”  $\chi^2$  statistic, i.e. one in which only pixels in which the model is statistically significant are included

**Parameters****reduced**

[bool] Return the reduced  $\chi^2$

**threshold**

[‘auto’ or ‘error’ or float] If ‘auto’, the threshold will be set to peak\_fraction \* the peak model value, where peak\_fraction is a kwarg passed to `get_model_xlimits` reflecting the fraction of the model peak to consider significant. If ‘error’, uses the error spectrum as the threshold

**kwargs**

[dict] passed to `get_model_xlimits()`

**Returns****chi2**

[float]  $\chi^2$  statistic or reduced  $\chi^2$  statistic ( $\chi^2/n$ )

$$\chi^2 = \sum ((d_i - m_i)^2 / e_i^2)$$

**peakbgfit**(*usemoments=True, annotate=None, vheight=True, height=0, negamp=None, fitype=None, renormalize=‘auto’, color=None, use\_lmfit=False, show\_components=None, debug=False, use\_window\_limits=True, guesses=None, nsigcut\_moments=None, plot=True, parinfo=None, \*\*kwargs*)

Fit a single peak (plus a background)

**Parameters****usemoments**

[bool] The initial guess will be set by the fitter’s ‘moments’ function (this overrides ‘guesses’)

**annotate**

[bool] Make a legend?

**vheight**

[bool] Fit a (constant) background as well as a peak?

**height**

[float] initial guess for background

**negamp**

[bool] If True, assumes amplitude is negative. If False, assumes positive. If None, can be either.

**fittype**

[bool] What function will be fit? fittype must have been Registryed in the peakbgfitters dict

**renormalize**

['auto' or bool] if 'auto' or True, will attempt to rescale small data ( $<1e-9$ ) to be closer to 1 (scales by the median) so that the fit converges better

**nsigcut\_moments**

[bool] pass to moment guesser; can do a sigma cut for moment guessing

**plot\_components**(*xarr=None*, *show\_hyperfine\_components=None*, *component\_yoffset=0.0*, *component\_lw=0.75*, *pars=None*, *component\_fit\_color='blue'*, *component\_kwargs={}*, *add\_baseline=False*, *plotkwargs={}, \*\*kwargs*)

Overplot the individual components of a fit

**Parameters****xarr**

[None] If none, will use the spectrum's xarr. Otherwise, plot the specified xarr. This is useful if you want to plot a well-sampled model when the input spectrum is undersampled

**show\_hyperfine\_components**

[None | bool] Keyword argument to pass to component codes; determines whether to return individual (e.g., hyperfine) components of a composite model

**component\_yoffset**

[float] Vertical (y-direction) offset to add to the components when plotting

**component\_lw**

[float] Line width of component lines

**component\_fitcolor**

[color] Color of component lines

**component\_kwargs**

[dict] Keyword arguments to pass to the `fitter.components` method

**add\_baseline**

[bool] Add the fit to the components before plotting. Makes sense to use if `self.Spectrum.baseline.subtracted == False`

**pars**

[parinfo] A parinfo structure or list of model parameters. If none, uses best-fit

**plot\_fit**(*xarr=None*, *annotate=None*, *show\_components=None*, *composite\_fit\_color='red'*, *lw=0.5*, *composite\_lw=0.75*, *pars=None*, *offset=None*, *use\_window\_limits=None*, *show\_hyperfine\_components=None*, *plotkwargs={}, \*\*kwargs*)

Plot the fit. Must have fitted something before calling this!

It will be automatically called whenever a spectrum is fit (assuming an axis for plotting exists)

kwargs are passed to the fitter's components attribute

**Parameters**

**xarr**

[None] If none, will use the spectrum's xarr. Otherwise, plot the specified xarr. This is useful if you want to plot a well-sampled model when the input spectrum is undersampled

**annotate**

[None or bool] Annotate the plot? If not specified, defaults to self.autoannotate

**show\_components**

[None or bool]

**show\_hyperfine\_components**

[None or bool] Show the individual gaussian components overlaid on the composite fit

**use\_window\_limits**

[None or bool] If False, will reset the window to include the whole spectrum. If True, leaves the window as is. Defaults to self.use\_window\_limits if None.

**pars**

[parinfo] A parinfo structure or list of model parameters. If none, uses best-fit

**offset**

[None or float] Y-offset. If none, uses the default self.Spectrum.plotter offset, otherwise, uses the specified float.

**plot\_model**(*pars*, *offset=0.0*, *annotate=False*, *clear=False*, *\*\*kwargs*)

Plot a model from specified input parameters (see plot\_fit for kwarg specification)

annotate is set to "false" because arbitrary annotations are not yet implemented

**plotresiduals**(*fig=2*, *axis=None*, *clear=True*, *color='k'*, *linewidth=0.5*, *drawstyle='steps-mid'*, *yoffset=0.0*, *label=True*, *pars=None*, *zeroline=None*, *set\_limits=True*, *\*\*kwargs*)

Plot residuals of the fit. Specify a figure or axis; defaults to figure(2).

**Parameters****fig**

[int] Figure number. Overridden by axis

**axis**

[axis] The axis to plot on

**pars**

[None or parlist] If set, the residuals will be computed for the input parameters

**zeroline**

[bool or None] Plot the "zero" line through the center of the residuals. If None, defaults to "True if yoffset!=0, False otherwise"

**kwargs are passed to matplotlib plot**

**print\_fit**(*print\_baseline=True*, *\*\*kwargs*)

Print the best-fit parameters to the command line

**refit**(*use\_lmfit=False*)

Redo a fit using the current parinfo as input

**register\_fitter**(*\*args*, *\*\*kwargs*)

Register a model fitter

Register a fitter function.

## Parameters

**name: string**

The fit function name.

**function: function**

The fitter function. Single-fitters should take `npars + 1` input parameters, where the +1 is for a 0th order baseline fit. They should accept an X-axis and data and standard fitting-function inputs (see, e.g., `gaussfitter`). Multi-fitters should take `N * npars`, but should also operate on X-axis and data arguments.

**npars: int**

How many parameters does the function being fit accept?

## Other Parameters

**override: True | False**

Whether to override any existing type if already present.

**key: char**

Key to select the fitter in interactive mode

**savefit()**

Save the fit parameters from a Gaussian fit to the FITS header

**selectregion**(*xmin=None, xmax=None, xtype='wcs', highlight=False, fit\_plotted\_area=True, reset=False, verbose=False, debug=False, use\_window\_limits=None, exclude=None, \*\*kwargs*)

Pick a fitting region in either WCS units or pixel units

## Parameters

**\*xmin / xmax\***

[[ float ]] The min/max X values to use in X-axis units (or pixel units if `xtype` is set). TAKES PRECEDENCE ALL OTHER BOOLEAN OPTIONS

**\*xtype\***

[[ string ]] A string specifying the `xtype` that `xmin/xmax` are specified in. It can be either 'wcs' or any valid `xtype` from `pyspeckit.spectrum.units`

**\*reset\***

[[ bool ]] Reset the selected region to the full spectrum? Only takes effect if `xmin` and `xmax` are not (both) specified. TAKES PRECEDENCE ALL SUBSEQUENT BOOLEAN OPTIONS

**\*fit\_plotted\_area\***

[[ bool ]] Use the plot limits *as specified in* :class: 'pyspeckit.spectrum.plotters'? Note that this is not necessarily the same as the window plot limits!

**\*use\_window\_limits\***

[[ bool ]] Use the plot limits *as displayed*. Defaults to `self.use_window_limits` (`pyspeckit.spectrum.interactive.use_window_limits`). Overwrites `xmin,xmax` set by plotter

**exclude: {list of length 2n,'interactive', None}**

- `interactive`: start an interactive session to select the include/exclude regions



- list: parsed as a series of (startpoint, endpoint) in the spectrum's X-axis units. Will exclude the regions between startpoint and endpoint
- None: No exclusion

**seterrspec**(*usestd=None, useresiduals=True*)

Simple wrapper function to set the error spectrum; will either use the input spectrum or determine the error using the RMS of the residuals, depending on whether the residuals exist.

**setfitspec**()

Set the spectrum that will be fit. This is primarily to remove NaNs from consideration: if you simply remove the data from both the X-axis and the Y-axis, it will not be considered for the fit, and a linear X-axis is not needed for fitting.

However, it may be possible to do this using masked arrays instead of setting errors to be 1e10...

**shift\_pars**(*frame=None*)

Shift the velocity / wavelength / frequency of the fitted parameters into a different frame

Right now this only takes care of redshift and only if redshift is defined. It should be extended to do other things later

**start\_interactive**(*debug=False, LoudDebug=False, reset\_selection=False, print\_message=True, clear\_all\_connections=True, \*\*kwargs*)

Initialize the interactive session

#### Parameters

**print\_message**

[bool] Print the interactive help message?

**clear\_all\_connections**

[bool] Clear all matplotlib event connections? (calls self.clear\_all\_connections())

**reset\_selection**

[bool] Reset the include mask to be empty, so that you're setting up a fresh region.

**xmax**

**xmin**

### 5.2.1 Fitting a user-defined model to a spectrum

damped\_lya\_profile is the function that generates the model and damped\_lya\_fitter creates the fitter class.

```
def damped_lya_profile(wave_to_fit, vs_n, am_n, fw_n, vs_b, am_b, fw_b, h1_col, h1_b,
                      h1_vel, d2h, resolution, single_component_flux=False,
                      return_components=False,
                      return_hyperfine_components=False):

    """
    Computes a damped Lyman-alpha profile (by calling the functions
    lya_intrinsic_profile_func and total_tau_profile_func) and convolves it
    to the proper resolution.

    """
```

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```

lya_intrinsic_profile = lya_intrinsic_profile_func(wave_to_fit,vs_n,am_n,fw_n,
                                                    vs_b,am_b,fw_b,single_component_flux=single_component_flux)
total_tau_profile = total_tau_profile_func(wave_to_fit,h1_col,h1_b,h1_vel,d2h)

lya_obs_high = lya_intrinsic_profile * total_tau_profile

## Convolution of the data ##
fw = lya_rest/resolution
aa = make_kernel(grid=wave_to_fit,fwhm=fw)
lyman_fit = np.convolve(lya_obs_high,aa,mode='same')

return lyman_fit*1e14

def damped_lya_fitter(multisingle='multi'):

    """
    Generator for Damped LyA fitter class

    """
    myclass = pyspeckit.models.model.SpectralModel(damped_lya_profile,
                                                    11,
                                                    parnames=['vs_n','am_n','fw_n','vs_b','am_b','fw_b','h1_col',
                                                                    'h1_b','h1_vel','d2h','resolution'],
                                                    parlimited=[(False,False),(True,False),(True,False),(False,False),
                                                                    (True,False),(True,False),(True,True),(True,True),
                                                                    (False,False),(True,True),(True,False)],
                                                    parlimits=[(14.4,14.6), (1e-16,0), (50.,0),(0,0), (1e-16,0),(50.,0),
                                                                    (17.0,19.5), (5.,20.), (0,0),(1.0e-5,2.5e-5),(10000.,0)])
    myclass.__name__ = "damped_lya"

    return myclass

## Load the spectrum, register the fitter, and fit
spec = pyspeckit.Spectrum(xarr=wave_to_fit, data=flux_to_fit*1e14,
                           error=error_to_fit*1e14, doplot=False,
                           header=spec_header)

spec.Registry.add_fitter('damped_lya',damped_lya_fitter(),11)

spec.specfit(fittype='damped_lya',
             guesses=[vs_n, am_n, fw_n, vs_b, am_b, fw_b, h1_col, h1_b,
                     h1_vel, d2h, resolution],
             quiet=False, fixed=[False, False, False, False, False,
                                 False, False, False, False, True, True])

## Check out the results
spec.specfit.parinfo.values
spec.specfit.parinfo.errors
reduced_chi2 = spec.specfit.chi2/spec.specfit.dof

```

## 5.3 Measurements

```
class pyspeckit.spectrum.measurements.Measurements(Spectrum, z=None, d=None, fluxnorm=None,
                                                    miscline=None, misctol=10.0, ignore=None,
                                                    derive=True, debug=False, restframe=False,
                                                    ptol=2, sort=False)
```

Bases: `object`

This can be called after a fit is run. It will inherit the `specfit` object and derive as much as it can from `modelpars`. Just do: `spec.measure(z, xunits, fluxnorm)`

Notes: If `z` (redshift) or `d` (distance) are present, we can compute integrated line luminosities rather than just fluxes. Provide distance in cm.

**Only works with Gaussians. To generalize:**

1. make sure we manipulate `modelpars` correctly, i.e. read in entries corresponding to wavelength/frequency/whatever correctly.

### Parameters

**z: float or None**  
redshift

**d: float or None**  
distance in cm (used for luminosities)

**fluxnorm: bool**  
Normalize the fluxes?

**miscline: dictionary**  
`miscline = [{'name': 'H_alpha', 'wavelength': 6565}]`

**misctol: tolerance (in Angstroms) for identifying an unmatched line**  
to the line(s) we specify in `miscline` dictionary.

**sort: bool**  
Sort the entries in order of observed wavelength (or velocity or frequency)

**bisection(*f, x\_guess*)**  
Find root of function using bisection method. Absolute tolerance of  $1e-4$  is being used.

**bracket\_root(*f, x\_guess, atol=0.0001*)**  
Bracket root by finding points where function goes from positive to negative.

**compute\_amplitude(*pars*)**  
Calculate amplitude of emission line. Should be easy - add multiple components if they exist. Currently assumes multiple components have the same centroid.

**compute\_flux(*pars*)**  
Calculate integrated flux of emission line. Works for multi-component fits too. Unnormalized.

**compute\_fwhm(*pars*)**  
Determine full-width at half maximum for multi-component fit numerically, or analytically if line has only a single component. Uses bisection technique for the former with absolute tolerance of  $1e-4$ .

**compute\_luminosity(*pars*)**  
Determine luminosity of line (need distance and flux units).

**derive()**  
Calculate luminosity and FWHM for all spectral lines.

**identify\_by\_position(*ptol*)**

Match observed lines to nearest reference line. Don't use spacing at all.

*ptol* = tolerance (in angstroms) to accept positional match

**identify\_by\_spacing()**

Determine identity of lines in `self.modelpars`. Fill entries of `self.lines` dictionary.

Note: This method will be infinitely slow for more than 10 or so lines.

**separate()**

For multicomponent lines, separate into broad and narrow components (assume only one of components is narrow).

**to\_tex()**

Write out fit results to tex format.

## 5.4 Units

Unit parsing and conversion tool. The `SpectroscopicAxis` class is meant to deal with unit conversion internally

Open Questions: Are there other FITS-valid projection types, unit types, etc. that should be included? What about for other fields (e.g., wavenumber?)

**class** `pyspeckit.spectrum.units.SpectroscopicAxis`

Bases: `astropy.units.quantity.Quantity`

A Spectroscopic Axis object to store the current units of the spectrum and allow conversion to other units and frames. Typically, units are velocity, wavelength, frequency, or redshift. Wavenumber is also hypothetically possible.

WARNING: If you index a `SpectroscopicAxis`, the resulting array will be a `SpectroscopicAxis` without a `dxarr` attribute! This can result in major problems; a workaround is being sought but subclassing numpy arrays is harder than I thought

Make a new spectroscopic axis instance Default units Hz

**as\_unit(*unit*, *equivalencies*=[], *velocity\_convention*=None, *refX*=None, *refX\_unit*=None, *center\_frequency*=None, *center\_frequency\_unit*=None, *\*\*kwargs*)**

Convert the spectrum to the specified units. This is a wrapper function to convert between frequency/velocity/wavelength and simply change the units of the X axis. Frame conversion is... not necessarily implemented.

**cdelt(*tolerance*=1e-08, *approx*=False)**

Return the channel spacing if channels are linear

**convert\_to\_unit(*unit*, *make\_dxarr*=True, *\*\*kwargs*)**

Return the X-array in the specified units without changing it Uses `as_unit` for the conversion, but changes internal values rather than returning them.

**coord\_to\_x(*xval*, *xunit*)**

Given an X-value assumed to be in the coordinate axes, return that value converted to *xunit* e.g.: `xarr.unit = 'km/s' xarr.refX = 5.0 xarr.refX_unit = GHz xarr.coord_to_x(6000,'GHz') == 5.1 # GHz`

**dxarr**

**classmethod** **find\_equivalencies(*velocity\_convention*=None, *center\_frequency*=None, *equivalencies*=[])**

Utility function to add equivalencies from the `velocity_convention` and the `center_frequency`

**in\_range**(*xval*)

Given an X coordinate in SpectroscopicAxis' units, return whether the pixel is in range

**make\_dxarr**(*coordinate\_location='center'*)

Create a “delta-x” array corresponding to the X array. It will have the same length as the input array, which is achieved by concatenating an extra pixel somewhere.

**refX**

**refX\_unit**

**refX\_units**

**set\_unit**(*unit, bad\_unit\_response='raise'*)

**umax**(*unit=None*)

Return the maximum value of the SpectroscopicAxis. If units specified, convert to those units first

**umin**(*unit=None*)

Return the minimum value of the SpectroscopicAxis. If units specified, convert to those units first

**units**

**classmethod validate\_unit**(*unit, bad\_unit\_response='raise'*)

**x\_to\_coord**(*xval, xunit, verbose=False*)

Given a wavelength/frequency/velocity, return the value in the SpectroscopicAxis's units e.g.: `xarr.unit = 'km/s' xarr.refX = 5.0 xarr.refX_unit = GHz xarr.x_to_coord(5.1,'GHz') == 6000 # km/s`

**x\_to\_pix**(*xval, xval\_unit=None, xval\_units=None, equivalencies=None*)

Given an X coordinate in SpectroscopicAxis' units, return the corresponding pixel number

**class** `pyspeckit.spectrum.units.SpectroscopicAxes`

Bases: `pyspeckit.spectrum.units.SpectroscopicAxis`

Counterpart to Spectra: takes a list of SpectroscopicAxis's and concatenates them while checking for consistency and maintaining header parameter

Make a new spectroscopic axis instance Default units Hz

## 5.5 Registration

PySpecKit is made extensible by allowing user-registered modules for reading, writing, and fitting data.

For examples of registration in use, look at the source code of `pyspeckit.spectrum.__init__` and `pyspeckit.spectrum.fitters`.

The registration functions can be accessed directly:

```
pyspeckit.register_reader
pyspeckit.register_writer
```

However, models are bound to individual instances of the Spectrum class, so they must be accessed via a specific instance

```
sp = pyspeckit.Spectrum('myfile.fits')
sp.specfit.register_fitter
```

Alternatively, you can access and edit the default Registry

```
pyspeckit.fitters.default_Registry.add_fitter
```

If you've already loaded a Spectrum instance, but then you want to reload fitters from the default\_Registry, or if you want to make your own Registry, you can use the semi-private method

```
MyRegistry = pyspeckit.fitters.Registry()
sp._register_fitters(registry=MyRegistry)
```

## 5.6 Examples

If you want to register a new variable-optical-depth deuterated ammonia model, you could do the following:

```
sp.specfit.register_fitter(name='nh2d', function=nh2d.nh2d_vtau_fitter, npars=4)
```

### 5.6.1 API

`pyspeckit.spectrum.__init__.register_reader(filetype, function, suffix, default=False)`  
Register a reader function.

#### Parameters

**filetype: str**

The file type name

**function: function**

The reader function. Should take a filename as input and return an X-axis object (see `units.py`), a spectrum, an error spectrum (initialize it to 0's if empty), and a pyfits header instance

**suffix: int**

What suffix should the file have?

`pyspeckit.spectrum.__init__.register_writer(filetype, function, suffix, default=False)`  
Register a writer function.

#### Parameters

**filetype: string**

The file type name

**function: function**

The writer function. Will be an attribute of Spectrum object, and called as `spectrum.Spectrum.write_hdf5()`, for example.

**suffix: int**

What suffix should the file have?

**class** `pyspeckit.spectrum.fitters.Registry`

This class is a simple wrapper to prevent fitter properties from being globals

**add\_fitter**(*name, function, npars, override=False, key=None, multisingle=None*)

Register a fitter function.

#### Parameters

**name: string**

The fit function name.

**function: function**

The fitter function. Single-fitters should take  $\text{npars} + 1$  input parameters, where the +1 is for a 0th order baseline fit. They should accept an X-axis and data and standard fitting-function inputs (see, e.g., `gaussfitter`). Multi-fitters should take  $N * \text{npars}$ , but should also operate on X-axis and data arguments.

**npars: int**

How many parameters does the function being fit accept?

#### Other Parameters

**override: True | False**

Whether to override any existing type if already present.

**key: char**

Key to select the fitter in interactive mode

## 5.7 Classes

### 5.7.1 spectrum

The spectrum module consists of the `Spectrum` class, with child classes `ObsBlock` and `Spectra` for multi-spectrum analysis of different types.

The `Spectrum` class is the main functional code. `ObsBlocks` are containers of multiple spectra of different objects. The `Spectra` class is a container of multiple spectra of the *same* object at different wavelengths/frequencies.

```
class pyspeckit.spectrum.classes.Spectrum(filename_or_magic=None, filetype=None, xarr=None,
                                         data=None, error=None, header=None, doplot=False,
                                         maskdata=True, unit=None, plotkwargs={}, xarrkwargs={},
                                         model_registry=None, filename=None,
                                         **kwargs)
```

Bases: `pyspeckit.spectrum.classes.SingleSpectrum`

The core class for the spectroscopic toolkit. Contains the data and error arrays along with wavelength / frequency / velocity information in various formats.

Create a `Spectrum` object.

Must either pass in a filename or ALL of `xarr`, `data`, and `header`, plus optionally `error`.

`kwargs` are passed to the file reader

#### Parameters

**filename\_or\_magic**

[string or something else] The filename or something with an `hdu` attribute. If `data`, `xarr`, and `error` are specified, leave filename blank.

**filetype**

[string] Specify the file type (only needed if it cannot be automatically determined from the filename)

**xarr**

[units.SpectroscopicAxis or np.ndarray] The X-axis of the data. If it is an np.ndarray, you must pass xarrkwargs or a valid header if you want to use any of the unit functionality.

**data**

[np.ndarray] The data array (must have same length as xarr)

**error**

[np.ndarray] The error array (must have same length as the data and xarr arrays)

**header**

[pyfits.Header or dict] The header from which to read unit information. Needs to be a pyfits.Header instance or another dictionary-like object with the appropriate information

**maskdata**

[boolean] turn the array into a masked array with all nan and inf values masked

**doplot**

[boolean] Plot the spectrum after loading it?

**plotkwargs**

[dict] keyword arguments to pass to the plotter

**xarrkwargs**

[dict] keyword arguments to pass to the SpectroscopicAxis initialization (can be used in place of a header)

**unit**

[str] The data unit

**filename**

[string] The file to read the spectrum from. If data, xarr, and error are specified, leave filename blank.

## Examples

```
>>> sp = pyspeckit.Spectrum(data=np.random.randn(100),
                             xarr=np.linspace(-50, 50, 100), error=np.ones(100)*0.1,
                             xarrkwargs={'unit': 'km/s', 'refX': 4.829, 'refX_unit': 'GHz',
                                           'xtype': 'VLSR-RAD'}, header={})
```

```
>>> xarr = pyspeckit.units.SpectroscopicAxis(np.linspace(-50, 50, 100),
                                              units='km/s', refX=6562.83, refX_unit='angstroms')
>>> data = np.random.randn(100)*5 + np.random.rand(100)*100
>>> err = np.sqrt(data/5.)*5. # Poisson noise
>>> sp = pyspeckit.Spectrum(data=data, error=err, xarr=xarr, header={})
```

```
>>> # if you already have a simple fits file
>>> sp = pyspeckit.Spectrum('test.fits')
```

**copy(deep=True)**

Create a copy of the spectrum with its own plotter, fitter, etc. Useful for, e.g., comparing smoothed to unsmoothed data



**crop**(*x1*, *x2*, *unit=None*, *\*\*kwargs*)

Replace the current spectrum with a subset from *x1* to *x2* in current units

Fixes CRPIX1 and baseline and model spectra to match cropped data spectrum

**data\_quantity**

**downsample**(*dsfactor*)

Downsample the spectrum (and all of its subsidiaries) without smoothing

**Parameters**

**dsfactor**

[int] Downsampling Factor

**error\_quantity**

**flux**

The data in the spectrum (flux = data, for compatibility with astropy’s Spectrum1D object).

**classmethod from\_hdu**(*hdu*)

Create a pyspeckit Spectrum object from an HDU

**classmethod from\_spectrum1d**(*spec1d*)

Tool to load a pyspeckit Spectrum from a specutils object

## Examples

```
>>> # grab many spectra from a multiextension FITS file
>>> spectra = specutils.io.fits.read_fits_spectrum1d('AAO.fits')
>>> sp = pyspeckit.Spectrum.from_spectrum1d(spectra[0])
```

```
>>> # open a single spectrum that could have been opened directly with pyspeckit
>>> spectrum = specutils.io.fits.read_fits_spectrum1d('gbt_1d.fits')
>>> sp = pyspeckit.Spectrum.from_spectrum1d(spectrum)
```

**getlines**(*linetype='radio'*, *\*\*kwargs*)

Access a registered database of spectral lines. Will add an attribute with the name *linetype*, which then has properties defined by the *speclines* module (most likely, a table and a “show” function to display the lines)

**interpnan**()

Interpolate over NAN values, replacing them with values interpolated from their neighbors using linear interpolation.

**measure**(*z=None*, *d=None*, *fluxnorm=None*, *miscline=None*, *misctol=10.0*, *ignore=None*, *derive=True*, *\*\*kwargs*)

Initialize the measurements class - only do this after you have run a fitter otherwise pyspeckit will be angry!

**moments**(*unit='km/s'*, *\*\*kwargs*)

Return the moments of the spectrum. In order to assure that the 1st and 2nd moments are meaningful, a ‘default’ unit is set. If unit is not set, will use current unit.

*Documentation imported from the moments module:*

Returns the gaussian parameters of a 1D distribution by calculating its moments. Depending on the input parameters, will only output a subset of the above.

Theory, from first principles (in the absence of noise):  $\text{integral}(\text{gaussian}) = \sqrt{2\pi}\sigma^2 * \text{amp}$   
 $\sigma = \text{integral} / \text{amp} / \sqrt{2\pi}$

In the presence of noise, this gets much more complicated. The noisy approach is inspired by [mpfit](#)

### Parameters

#### **Xax**

[np.ndarray] The x-axis for computing the 1st and 2nd moments

#### **data**

[np.ndarray] The data from which to compute the various moments

#### **estimator**

[function] A function to estimate the “height” or “background level” of the data, e.g. mean or median. If masked arrays are being used, use the np.ma versions of the numpy functions

#### **negamp: bool or None**

Force the peak negative (True), positive (False), or the sign of the peak will be “autodetected” (negamp=None)

#### **nsigcut: float or None**

If specified, the code will attempt to estimate the noise and only use data above/below n-sigma above the noise. The noise will be estimated from the data unless the noise is specified with noise\_estimate

#### **noise\_estimate: float or None**

Guess for the noise value. Only matters if nsigcut is specified.

#### **vheight**

[bool] Include an estimate of the background level?

### Returns

(height, amplitude, x, width\_x)

#### **height**

[float] is the background level

#### **amplitude**

[float] is the maximum (or minimum) of the data after background subtraction

#### **x**

[float] is the first moment

#### **width\_x**

[float] is the second moment

#### **parse\_hdf5\_header(hdr)**

HDF5 reader will create a hdr dictionary from HDF5 dataset attributes if they exist. This routine will convert that dict to a pyfits header instance.

#### **parse\_header(hdr, specname=None)**

Parse parameters from a .fits header into required spectrum structure parameters

#### **parse\_text\_header(Table)**

Grab relevant parameters from a table header (xaxis type, etc)

This function should only exist for Spectrum objects created from .txt or other atpy table type objects

#### **shape**

Return the data shape (a property of the Spectrum)

**slice**(*start=None, stop=None, unit='pixel', copy=True, xcopy=True, preserve\_fits=False*)

Slicing the spectrum

**Warning:** this is the same as cropping right now, but it returns a copy instead of cropping inplace

#### **Parameters**

##### **start**

[numpy.float or int or astropy quantity] start of slice

##### **stop**

[numpy.float or int or astropy quantity] stop of slice

##### **unit**

[str] allowed values are any supported physical unit, 'pixel'

##### **copy**

[bool] Return a 'view' of the data or a copy?

##### **preserve\_fits**

[bool] Save the fitted parameters from self.fitter?

**smooth**(*smooth, downsample=True, \*\*kwargs*)

Smooth the spectrum by factor [smooth](#).

Documentation from the `smooth` module:

sm.smooth doc:

Smooth and downsample the data array. NaN data points will be replaced with interpolated values

#### **Parameters**

##### **smooth**

[float] Number of pixels to smooth by

##### **smoothtype**

[[ 'gaussian', 'hanning', or 'boxcar' ]] type of smoothing kernel to use

##### **downsample**

[bool] Downsample the data?

##### **downsample\_factor**

[int] Downsample by the smoothing factor, or something else?

##### **convmode**

[[ 'full', 'valid', 'same' ]] see `numpy.convolve`. 'same' returns an array of the same length as 'data' (assuming data is larger than the kernel)

**stats**(*statrange=(), interactive=False*)

Return some statistical measures in a dictionary (somewhat self-explanatory)

## Parameters

### **statrange**

[2-element tuple] X-range over which to perform measures

### **interactive**

[bool] specify range interactively in plotter

### **unit**

### **units**

**write**(*filename*, *type=None*, *\*\*kwargs*)

Write the spectrum to a file. The available file types are listed in `spectrum.writers.writers`

*type* - what type of file to write to? If not specified, will attempt to determine type from suffix

**class** `pyspeckit.spectrum.classes.Spectra`(*speclist*, *xunit=None*, *model\_registry=None*, *\*\*kwargs*)

Bases: `pyspeckit.spectrum.classes.BaseSpectrum`

A list of individual Spectrum objects. Intended to be used for concatenating different wavelength observations of the SAME OBJECT. Can be operated on just like any Spectrum object, including fitting. Useful for fitting multiple lines on non-contiguous axes simultaneously. Be wary of plotting these though...

Can be indexed like python lists.

X array is forcibly sorted in increasing order

**fiteach**(*\*\*kwargs*)

Fit each spectrum within the Spectra object

**classmethod** `from_spectrum1d_list`(*lst*)

Tool to load a collection of pyspeckit Spectra from a specutils list of Spectrum1D objects

## Examples

```
>>> # grab many spectra from a multiextension FITS file
>>> spectra = specutils.io.fits.read_fits_spectrum1d('AAO.fits')
>>> sp = pyspeckit.Spectrum.from_spectrum1d_list(spectra)
```

**ploteach**(*xunit=None*, *inherit\_fit=False*, *plot\_fit=True*, *plotfitkwargs={}*, *\*\*plotkwargs*)

Plot each spectrum in its own window *inherit\_fit* - if specified, will grab the fitter & fitter properties from Spectra

**smooth**(*smooth*, *\*\*kwargs*)

Smooth the spectrum by factor “smooth”. Options are defined in `sm.smooth`

because ‘Spectra’ does not have a header attribute, don’t do anything to it...

**class** `pyspeckit.spectrum.classes.ObsBlock`(*speclist*, *xtype='frequency'*, *xarr=None*, *force=False*, *model\_registry=None*, *\*\*kwargs*)

Bases: `pyspeckit.spectrum.classes.Spectra`

An Observation Block

Consists of multiple spectra with a shared X-axis. Intended to hold groups of observations of the same object in the same setup for later averaging.

ObsBlocks can be indexed like python lists.

**average**(*weight=None, inverse\_weight=False, error='erravgtrn', debug=False*)

Average all scans in an ObsBlock. Returns a single Spectrum object

#### Parameters

**weight**

[string] a header keyword to weight by. If not specified, the spectra will be averaged without weighting

**inverse\_weight**

[bool] Is the header keyword an inverse-weight (e.g., a variance?)

**error**

[[‘scanrms’, ‘erravg’, ‘erravgtrn’]] estimate the error spectrum by one of three methods. ‘scanrms’ : the standard deviation of each pixel across all scans ‘erravg’ : the average of all input error spectra ‘erravgtrn’ : the average of all input error spectra divided by  $\sqrt{n\_obs}$

**smooth**(*smooth, \*\*kwargs*)

Smooth the spectrum by factor “smooth”. Options are defined in sm.smooth

pyspeckit.spectrum.**register\_reader**(*filetype, function, suffix, default=False*)

Register a reader function.

#### Parameters

**filetype: str**

The file type name

**function: function**

The reader function. Should take a filename as input and return an X-axis object (see units.py), a spectrum, an error spectrum (initialize it to 0’s if empty), and a pyfits header instance

**suffix: int**

What suffix should the file have?

pyspeckit.spectrum.**register\_writer**(*filetype, function, suffix, default=False*)

Register a writer function.

#### Parameters

**filetype: string**

The file type name

**function: function**

The writer function. Will be an attribute of Spectrum object, and called as spectrum.Spectrum.write\_hdf5(), for example.

**suffix: int**

What suffix should the file have?

## 5.7.2 Cubes

Pyspeckit can do a few things with spectral cubes. The most interesting is the spectral line fitting.

Cube objects have a `fiteach()` method that will fit each spectral line within a cube. It can be made to do this in parallel with the multicore option.

As of version 0.16, pyspeckit cubes can be read from `SpectralCube` objects:

```
>>> pcube = pyspeckit.Cube(cube=mySpectralCube)
```

Otherwise, they can be created from FITS cubes on disk:

```
>>> pcube = pyspeckit.Cube(filename="mycube.fits")
```

or from arrays:

```
>>> mycube = np.random.randn(250,50,50)
>>> myxaxis = np.linspace(-100,100,250)
>>> pcube = pyspeckit.Cube(cube=mycube, xarr=myxaxis, xunit='km/s')
```

The most interesting features of the `Cube` object are the `fiteach()` method, which fits a model spectrum to each element of the cube, and `mapplot`, which plots up various projections of the cube.

`Cube.mapplot` will create an interactive plot window. You can click on any pixel shown in that window and pull up a second window showing the spectrum at that pixel. If you've fitted the cube, the associated best-fit model will also be shown. This interactive setup can be a bit fragile, though, so please report bugs aggressively so we can weed them out!

The interactive viewer has a few button interactions described [here](#).

## Cubes

Tools to deal with spectroscopic data cubes.

Some features in Cubes require additional packages:

- smoothing - requires `agpy`'s `smooth` and `parallel_map` routines
- `pyregion`

The 'grunt work' is performed by the `cubes` module

```
class pyspeckit.cubes.SpectralCube.Cube(filename=None, cube=None, xarr=None, xunit=None, errorcube=None, header=None, x0=0, y0=0, maskmap=None,
                                         **kwargs)
```

Bases: `pyspeckit.spectrum.classes.Spectrum`

A pyspeckit Cube object. Can be created from a FITS file on disk or from an array or a `spectral_cube.SpectralCube` object. If an array is used to instantiate the cube, the `xarr` keyword must be given, specifying the X-axis units

### Parameters

#### filename

[str, optional] The name of a FITS file to open and read from. Must be 3D

#### cube

[`np.ndarray`, `spectral_cube.SpectralCube`, or `astropy.units.Quantity`] The data from which to instantiate a Cube object. If it is an array or an astropy Quantity (which is an array with attached units), the X-axis must be specified. If this is given as a `SpectralCube` object, the X-axis and units should be handled automatically.

#### xarr

[`np.ndarray` or `astropy.units.Quantity`, optional] The X-axis of the spectra from each cube. This actually corresponds to axis 0, or what we normally refer to as the Z-axis of the

cube, but it indicates the X-axis in a plot of intensity vs wavelength. The units for this array are specified in the `xunit` keyword unless a `Quantity` is given.

#### **xunit**

[str, optional] The unit of the `xarr` array if `xarr` is given as a numpy array

#### **errorcube**

[np.ndarray, `spectral_cube.SpectralCube`, or `Quantity`, optional] A cube with the same shape as the input cube providing the 1-sigma error for each voxel. This can be specified more efficiently as an error map for most use cases, but that approach has not yet been implemented. However, you can pass a 2D error map to `fiteach`.

#### **header**

[`fits.Header` or dict, optional] The header associated with the data. Only needed if the cube is given as an array or a quantity.

#### **x0, y0**

[int] The initial spectrum to use. The `Cube` object can be treated as a `pyspeckit.Spectrum` object, with all the associated tools (plotter, fitter) using the `set_spectrum` method to select a pixel from the cube to plot and fit. However, it is generally more sensible to extract individual spectra and treat them separately using the `get_spectrum` method, so these keywords MAY BE DEPRECATED in the future.

#### **maskmap**

[np.ndarray, optional] A boolean mask map, where True implies that the data are good. This will be used for both plotting using `mapplot` and fitting using `fiteach`.

#### **copy(*deep=True*)**

Create a copy of the spectral cube with its own plotter, fitter, etc. Useful for, e.g., comparing smoothed to unsmoothed data

#### **crop(*x1, x2, unit=None, \*\*kwargs*)**

Replace the current spectrum with a subset from `x1` to `x2` in current units

Fixes CRPIX1 and baseline and model spectra to match cropped data spectrum

#### **data\_quantity**

#### **downsample(*dsfactor*)**

Downsample the spectrum (and all of its subsidiaries) without smoothing

#### **Parameters**

##### **dsfactor**

[int] Downsampling Factor

#### **error\_quantity**

**fiteach**(*errspec=None, errmap=None, guesses=(), verbose=True, verbose\_level=1, quiet=True, signal\_cut=3, usemomentcube=None, blank\_value=0, integral=False, direct\_integral=False, absorption=False, use\_nearest\_as\_guess=False, use\_neighbor\_as\_guess=False, start\_from\_point=(0, 0), multicore=1, position\_order=None, continuum\_map=None, prevalidate\_guesses=False, maskmap=None, \*\*fitkwargs*)

Fit a spectrum to each valid pixel in the cube

For guesses, priority is `use_nearest_as_guess`, `usemomentcube`, `guesses`, None

Once you have successfully run this function, the results will be stored in the `.parcube` and `.errcube` attributes, which are each cubes of shape `[npars, ny, nx]`, where `npars` is the number of fitted parameters

and `nx`, `ny` are the shape of the map. `errcube` contains the errors on the fitted parameters (1-sigma, as returned from the Levenberg-Marquardt fit's covariance matrix). You can use the attribute `has_fit`, which is a map of shape `[ny, nx]` to find which pixels have been successfully fit.

### Parameters

**use\_nearest\_as\_guess: bool**

Unless the fitted point is the first, it will find the nearest other point with a successful fit and use its best-fit parameters as the guess

**use\_neighbor\_as\_guess: bool**

Set this keyword to use the average best-fit parameters from neighboring positions with successful fits as the guess

**start\_from\_point: tuple(int,int)**

Either start from the center or from a point defined by a tuple. Work outward from that starting point.

**position\_order: ndarray[naxis=2]**

2D map of region with pixel values indicating the order in which to carry out the fitting. Any type with increasing pixel values.

**guesses: tuple or ndarray[naxis=3]**

Either a tuple/list of guesses with `len(guesses) = npars` or a cube of guesses with shape `[npars, ny, nx]`. NOT TRUE, but a good idea in principle: You can also use a dictionary of the form `{(y,x): [list of length npars]}`, where `(y,x)` specifies a pixel location. If the dictionary method is used, `npars` must be specified and it sets the length of the first parameter axis

**signal\_cut: float**

Minimum signal-to-noise ratio to “cut” on (i.e., if peak in a given spectrum has `s/n` less than this value, ignore it)

**blank\_value: float**

Value to replace non-fitted locations with. A good alternative is `numpy.nan`

**errmap: ndarray[naxis=2] or ndarray[naxis=3]**

A map of errors used for the individual pixels of the spectral cube. 2D `errmap` results in an equal weighting of each given spectrum, while a 3D array sets individual weights of each channel

**verbose: bool**

**verbose\_level: int**

Controls how much is output. 0,1 - only changes frequency of updates in loop 2 - print out messages when skipping pixels 3 - print out messages when fitting pixels 4 - specfit will be verbose

**multicore: int**

if `>1`, try to use multiprocessing via `parallel_map` to run on multiple cores

**continuum\_map: np.ndarray**

Same shape as error map. Subtract this from data before estimating noise.

**prevalidate\_guesses: bool**

An extra check before fitting is run to make sure the guesses are all within the specified limits. May be slow, so it is off by default. It also should not be necessary, since careful checking is performed before each fit.



**maskmap**

[np.ndarray, optional] A boolean mask map, where True implies that the data are good. This will be used for both plotting using `mapplot` and fitting using `fiteach`. If None, will use `self.maskmap`.

**integral**

[bool] If set, the integral of each spectral fit will be computed and stored in the attribute `.integralmap`

**direct\_integral**

[bool] Return the integral of the *spectrum* (as opposed to the fitted model) over a range defined by the `integration_limits` if specified or `threshold` otherwise

**flux**

The data in the spectrum (`flux = data`, for compatibility with `astropy`'s `Spectrum1D` object).

**classmethod from\_hdu(hdu)**

Create a `pyspeckit Spectrum` object from an HDU

**classmethod from\_spectrum1d(spec1d)**

Tool to load a `pyspeckit Spectrum` from a `specutils` object

**Examples**

```
>>> # grab many spectra from a multiextension FITS file
>>> spectra = specutils.io.fits.read_fits_spectrum1d('AAO.fits')
>>> sp = pyspeckit.Spectrum.from_spectrum1d(spectra[0])
```

```
>>> # open a single spectrum that could have been opened directly with pyspeckit
>>> spectrum = specutils.io.fits.read_fits_spectrum1d('gbt_1d.fits')
>>> sp = pyspeckit.Spectrum.from_spectrum1d(spectrum)
```

**get\_apspec(aperture, coordsys=None, method='mean', \*\*kwargs)**

Extract an aperture using `cubes.extract_aperture` (defaults to Cube pixel coordinates)

**aperture [tuple or list] (x, y, radius)**

The aperture to use when extracting the data

**coordsys [ 'celestial' | 'galactic' | None]**

the coordinate system the aperture is specified in None indicates pixel coordinates (default)

**wunit [str]**

arcsec, arcmin, or degree

**get\_modelcube(update=False, multicore=1)**

Return or generate a “model cube”, which will have the same shape as the `.cube` but will have spectra generated from the fitted model.

If the model cube does not yet exist, one will be generated

**Parameters****update**

[bool] If the cube has already been computed, set this to True to recompute the model.

**multicore: int**

if >1, try to use multiprocessing via `parallel_map` to run on multiple cores

**get\_spectrum**(*x, y*)

Very simple: get the spectrum at coordinates *x,y*

(inherits fitter from self)

Returns a SpectroscopicAxis instance

**get\_lines**(*linetype='radio', \*\*kwargs*)

Access a registered database of spectral lines. Will add an attribute with the name *linetype*, which then has properties defined by the *speclines* module (most likely, a table and a “show” function to display the lines)

**interp\_nans**()

Interpolate over NAN values, replacing them with values interpolated from their neighbors using linear interpolation.

**load\_fits**(*fitsfile*)

**load\_model\_fit**(*fitsfilename, npars, npeaks=1, fitype=None, \_temp\_fit\_loc=(0, 0)*)

Load a parameter + error cube into the *.parcube* and *.errcube* attributes. The models can then be examined and plotted using *.mapplot* as if you had run *.fiteach*.

#### Parameters

**fitsfilename**

[str] The filename containing the parameter cube written with *write\_fit*

**npars**

[int] The number of parameters in the model fit for a single spectrum

**npeaks**

[int] The number of independent peaks fit toward each spectrum

**fitype**

[str, optional] The name of the fitype, e.g. ‘gaussian’ or ‘voigt’, from the pyspeckit fitter registry. This is optional; it should have been written to the FITS header and will be read from there if it is not specified

**\_temp\_fit\_loc**

[tuple (int,int)] The initial spectrum to use to generate components of the class. This should not need to be changed.

**load\_spectral\_cube**(*cube*)

Load the cube from a *spectral\_cube.SpectralCube* object

**measure**(*z=None, d=None, fluxnorm=None, miscline=None, misctol=10.0, ignore=None, derive=True, \*\*kwargs*)

Initialize the measurements class - only do this after you have run a fitter otherwise pyspeckit will be angry!

**moment\_each**(*verbose=True, verbose\_level=1, multicore=1, \*\*kwargs*)

Return a cube of the moments of each pixel

#### Parameters

**multicore: int**

if >1, try to use multiprocessing via *parallel\_map* to run on multiple cores

**moments**(*unit='km/s', \*\*kwargs*)

Return the moments of the spectrum. In order to assure that the 1st and 2nd moments are meaningful, a ‘default’ unit is set. If unit is not set, will use current unit.

*Documentation imported from the moments module:*

Returns the gaussian parameters of a 1D distribution by calculating its moments. Depending on the input parameters, will only output a subset of the above.

Theory, from first principles (in the absence of noise):  $\text{integral}(\text{gaussian}) = \sqrt{2\pi}\sigma^2 * \text{amp}$   
 $\sigma = \text{integral} / \text{amp} / \sqrt{2\pi}$

In the presence of noise, this gets much more complicated. The noisy approach is inspired by [mpfit](#)

### Parameters

#### **Xax**

[np.ndarray] The x-axis for computing the 1st and 2nd moments

#### **data**

[np.ndarray] The data from which to compute the various moments

#### **estimator**

[function] A function to estimate the “height” or “background level” of the data, e.g. mean or median. If masked arrays are being used, use the np.ma versions of the numpy functions

#### **negamp: bool or None**

Force the peak negative (True), positive (False), or the sign of the peak will be “autodetected” (negamp=None)

#### **nsigcut: float or None**

If specified, the code will attempt to estimate the noise and only use data above/below n-sigma above the noise. The noise will be estimated from the data unless the noise is specified with noise\_estimate

#### **noise\_estimate: float or None**

Guess for the noise value. Only matters if nsigcut is specified.

#### **vheight**

[bool] Include an estimate of the background level?

### Returns

**(height, amplitude, x, width\_x)**

#### **height**

[float] is the background level

#### **amplitude**

[float] is the maximum (or minimum) of the data after background subtraction

#### **x**

[float] is the first moment

#### **width\_x**

[float] is the second moment

#### **parse\_hdf5\_header(hdr)**

HDF5 reader will create a hdr dictionary from HDF5 dataset attributes if they exist. This routine will convert that dict to a pyfits header instance.

**parse\_header**(*hdr, specname=None*)

Parse parameters from a .fits header into required spectrum structure parameters

**parse\_text\_header**(*Table*)

Grab relevant parameters from a table header (xaxis type, etc)

This function should only exist for Spectrum objects created from .txt or other atpy table type objects

**plot\_apspec**(*aperture, coordsys=None, reset\_ylimits=True, wunit='arcsec', method='mean', \*\*kwargs*)

Extract an aperture using cubes.extract\_aperture (defaults to Cube coordinates)

#### Parameters

**aperture**

[list]

A list of aperture parameters, e.g.

- For a circular aperture, len(ap)=3: + ap = [xcen,ycen,radius]
- For an elliptical aperture, len(ap)=5: + ap = [xcen,ycen,height,width,PA]

**coordsys**

[None or str] The coordinate system of the aperture (e.g., galactic, fk5, None for pixel)

**method**

['mean' or 'sum'] Either average over parallel spectra or sum them.

**plot\_fit**(*x, y, silent=False, \*\*kwargs*)

If fiteach has been run, plot the best fit at the specified location

#### Parameters

**x**

[int]

**y**

[int] The x, y coordinates of the pixel (indices 2 and 1 respectively in numpy notation)

**plot\_spectrum**(*x, y, plot\_fit=False, \*\*kwargs*)

Fill the .data array with a real spectrum and plot it

**set\_apspec**(*aperture, coordsys=None, method='mean'*)

Extract an aperture using cubes.extract\_aperture (defaults to Cube coordinates)

**set\_spectrum**(*x, y*)

**shape**

Return the data shape (a property of the Spectrum)

**show\_fit\_param**(*parnumber, \*\*kwargs*)

If pars have been computed, display them in the mapplot window

#### Parameters

**parnumber**

[int] The index of the parameter in the parameter cube

**show\_moment**(*momentnumber*, *\*\*kwargs*)

If moments have been computed, display them in the mapplot window

**slice**(*start=None*, *stop=None*, *unit='pixel'*, *preserve\_fits=False*, *copy=True*, *update\_header=False*)

Slice a cube along the spectral axis (equivalent to “spectral\_slab” from the spectral\_cube package)

#### Parameters

**start**

[numpy.float or int] start of slice

**stop**

[numpy.float or int] stop of slice

**unit**

[str] allowed values are any supported physical unit, ‘pixel’

**update\_header**

[bool] modifies the header of the spectral cube according to the slice

**smooth**(*factor*, *\*\*kwargs*)

Smooth the spectrum by factor *factor*.

Documentation from the `cubes.spectral_smooth` module:

**stats**(*statrange=()*, *interactive=False*)

Return some statistical measures in a dictionary (somewhat self-explanatory)

#### Parameters

**statrange**

[2-element tuple] X-range over which to perform measures

**interactive**

[bool] specify range interactively in plotter

**unit**

**units**

**write**(*filename*, *type=None*, *\*\*kwargs*)

Write the spectrum to a file. The available file types are listed in `spectrum.writers.writers`

*type* - what type of file to write to? If not specified, will attempt to determine type from suffix

**write\_cube**()

**write\_fit**(*fitcubefilename*, *overwrite=False*)

Write out a fit cube containing the `.parcube` and `.errcube` using the information in the fit’s `parinfo` to set the header keywords. The `PLANE#` keywords will be used to indicate the content of each plane in the data cube written to the FITS file. All of the fitted parameters will be written first, followed by all of the errors on those parameters. So, for example, if you have fitted a single gaussian to each pixel, the dimensions of the saved cube will be `[6, ny, nx]`, and they will be the amplitude, centroid, width, error on amplitude, error on centroid, and error on width, respectively.

To load such a file back in for plotting purposes, see `SpectralCube.load_model_fit`.

#### Parameters

**fitcubefilename: string**

Filename to write to

**overwrite: bool**

Overwrite file if it exists?

**class** pyspeckit.cubes.SpectralCube.**CubeStack**(*cubelist*, *xunit*='GHz', *x0*=0, *y0*=0, *maskmap*=None, *\*\*kwargs*)

Bases: [pyspeckit.cubes.SpectralCube.Cube](#)

The Cube equivalent of Spectra: for stitching multiple cubes with the same spatial grid but different frequencies together

Initialize the Cube. Accepts FITS files.

x0,y0 - initial spectrum to use (defaults to lower-left corner)

## MapPlot

Make plots of the cube and interactively connect them to spectrum plotting. This is really an interactive component of the package; nothing in here is meant for publication-quality plots, but more for user interactive analysis.

That said, the plotter makes use of [APLpy](#), so it is possible to make publication-quality plots.

**author**

Adam Ginsburg

**date**

03/17/2011

---

**class** pyspeckit.cubes.mapplot.**MapPlotter**(*Cube*=None, *figure*=None, *doplot*=False, *\*\*kwargs*)

Bases: [object](#)

Class to plot a spectrum

See [mapplot](#) for use documentation; this docstring is only for initialization.

Create a map figure for future plotting

**circle**(*x1*, *y1*, *x2*, *y2*, *\*\*kwargs*)

Plot the spectrum of a circular aperture

**click**(*event*)

Record location of downclick

**copy**(*parent*=None)

Create a copy of the map plotter with blank (uninitialized) axis & figure

[ **parent** ]

A spectroscopic axis instance that is the parent of the specfit instance. This needs to be specified at some point, but defaults to None to prevent overwriting a previous plot.

**makeplane**(*estimator*=<function nanmean>)

Create a “plane” view of the cube, either by slicing or projecting it or by showing a slice from the best-fit model parameter cube.

**Parameters**

**estimator**

[[ function | 'max' | 'int' | FITS filename | integer | slice ]] A non-pythonic, non-duck-typed variable. If it's a function, apply that function along the cube's spectral axis to obtain an estimate (e.g., mean, min, max, etc.). 'max' will do the same thing as passing np.max 'int' will attempt to integrate the image (which is why I didn't duck-type) (integrate means sum and multiply by dx) a .fits filename will be read using pyfits (so you can make your own cover figure) an integer will get the n'th slice in the parcube if it exists If it's a slice, slice the input data cube along the Z-axis with this slice

**mapplot**(*convention*='calabretta', *colorbar*=True, *useaplpy*=True, *vmin*=None, *vmax*=None, *cmap*=None, *plotkwargs*={}, \*\*kwargs)

Plot up a map based on an input data cube.

The map to be plotted is selected using [makeplane](#). The estimator keyword argument is passed to that function.

The plotted map, once shown, is interactive. You can click on it with any of the three mouse buttons.

**Button 1 or keyboard '1':**

Plot the selected pixel's spectrum in another window. Mark the clicked pixel with an 'x'

**Button 2 or keyboard 'o':**

Overplot a second (or third, fourth, fifth...) spectrum in the external plot window

**Button 3:**

Disconnect the interactive viewer

You can also click-and-drag with button 1 to average over a circular region. This same effect can be achieved by using the 'c' key to set the /c/enter of a circle and the 'r' key to set its /r/radius (i.e., hover over the center and press 'c', then hover some distance away and press 'r').

**Parameters****convention**

['calabretta' or 'griesen'] The default projection to assume for Galactic data when plotting with aplpy.

**colorbar**

[bool] Whether to show a colorbar

**plotkwargs**

[dict, optional] A dictionary of keyword arguments to pass to aplpy.show\_colorscale or matplotlib.pyplot.imshow

**useaplpy**

[bool] Use aplpy if a FITS header is available

**vmin, vmax: float or None**

Override values for the vmin/vmax values. Will be automatically determined if left as None

**.. todo:**

Allow mapplot in subfigure

**plot\_spectrum**(*event*, *plot\_fit*=True)

Connects map cube to Spectrum...

**refresh**()

## cubes.py

From `agpy`, contains functions to perform various transformations on data cubes and their headers.

`pyspeckit.cubes.cubes.aper_world2pix(ap, wcs, coordsys='galactic', wunit='arcsec')`

Converts an elliptical aperture (x,y,width,height,PA) from WCS to pixel coordinates given an input wcs (an instance of the `pywcs.WCS` class). Must be a 2D WCS header.

`pyspeckit.cubes.cubes.baseline_cube(cube, polyorder=None, cubemask=None, splineorder=None, numcores=None, sampling=1)`

Given a cube, fit a polynomial to each spectrum

### Parameters

**cube: np.ndarray**

An ndarray with `ndim = 3`, and the first dimension is the spectral axis

**polyorder: int**

Order of the polynomial to fit and subtract

**cubemask: boolean ndarray**

Mask to apply to cube. Values that are True will be ignored when fitting.

**numcores**

[None or int] Number of cores to use for parallelization. If None, will be set to the number of available cores.

`pyspeckit.cubes.cubes.blfunc_generator(x=None, polyorder=None, splineorder=None, sampling=1)`

Generate a function that will fit a baseline (polynomial or spline) to a data set. Either `splineorder` or `polyorder` must be set

### Parameters

**x**

[np.ndarray or None] The X-axis of the fitted array. Will be set to `np.arange(len(data))` if not specified

**polyorder**

[None or int] The polynomial order.

**splineorder**

[None or int]

**sampling**

[int] The sampling rate to use for the data. Can set to higher numbers to effectively down-sample the data before fitting

`pyspeckit.cubes.cubes.coords_in_image(fitsfile, lon, lat, system='galactic')`

Determine whether the coordinates are inside the image

`pyspeckit.cubes.cubes.extract_aperture(cube, ap, r_mask=False, wcs=None, coordsys='galactic', wunit='arcsec', debug=False, method='mean')`

Extract an aperture from a data cube. E.g. to acquire a spectrum of an outflow that is extended.

Cube should have shape [z,y,x], e.g. `cube = fits.getdata('datacube.fits')`

Apertures are specified in PIXEL units with an origin of 0,0 (NOT the 1,1 fits standard!) unless `wcs` and `coordsys` are specified

### Parameters



**ap**

[list]

**For a circular aperture, len(ap)=3:**

ap = [xcen,ycen,radius]

**For an elliptical aperture, len(ap)=5:**

ap = [xcen,ycen,height,width,PA]

**wcs**

[wcs] a pywcs.WCS instance associated with the data cube

**coordsys**

[str] the coordinate system the aperture is specified in. Options are 'celestial' and 'galactic'.

Default is 'galactic'

**wunit**

[str] units of width/height. default 'arcsec', options 'arcmin' and 'degree'

**method**

[str] 'mean' or 'sum' (average over spectra, or sum them) or 'error' for sqrt(sum-of-squares / n)

**Other Parameters****r\_mask**

[bool]

**return mask in addition to spectrum (for error checking?)**pyspeckit.cubes.cubes.**flatten\_header**(*header, delete=False*)

Attempt to turn an N-dimensional fits header into a 2-dimensional header Turns all CRPIX[&gt;2] etc. into new keywords with suffix 'A'

header must be a fits.Header instance

pyspeckit.cubes.cubes.**getspec**(*lon, lat, rad, cube, header, r\_fits=True, inherit=True, wunit='arcsec'*)

Given a longitude, latitude, aperture radius (arcsec), and a cube file, return a .fits file or a spectrum.

**Parameters****lon: float****lat: float**

longitude and latitude center of a circular aperture in WCS coordinates must be in coordinate system of the file

**rad: float**

radius (default degrees) of aperture

pyspeckit.cubes.cubes.**getspec\_reg**(*cubefilename, region, \*\*kwargs*)

Aperture extraction from a cube using a pyregion circle region

The region must be in the same coordinate system as the cube header

**Warning:** The second argument of getspec\_reg requires a pyregion region list, and therefore this code depends on [pyregion](#).

`pyspeckit.cubes.cubes.integ(file, vrange, xcen=None, xwidth=None, ycen=None, ywidth=None, **kwargs)`

wrapper of `subimage_integ` that defaults to using the full image

`pyspeckit.cubes.cubes.plane_smooth(cube, cubedim=0, parallel=True, numcores=None, **kwargs)`  
parallel-map the smooth function

### Parameters

#### **parallel: bool**

defaults True. Set to false if you want serial (for debug purposes?)

#### **numcores: int**

pass to `parallel_map` (None = use all available)

`pyspeckit.cubes.cubes.speccen_header(header, lon=None, lat=None, proj='TAN', system='celestial', spectral_axis=3, celestial_axes=[1, 2])`

Turn a cube header into a spectrum header, retaining RA/Dec vals where possible (speccen is like flatten; spec-ify would be better but, specify? nah)

Assumes 3rd axis is velocity

`pyspeckit.cubes.cubes.spectral_smooth(cube, smooth_factor, downsample=True, parallel=True, numcores=None, **kwargs)`

Smooth the cube along the spectral direction

`pyspeckit.cubes.cubes.subcube(cube, xcen, xwidth, ycen, ywidth, header=None, dvmult=False, return_HDU=False, units='pixels', widthunits='pixels')`

Crops a data cube

All units assumed to be pixel units

cube has dimensions (velocity, y, x)

xwidth and ywidth are “radius” values, i.e. half the length that will be extracted

if dvmult is set, multiple the average by DV (this is useful if you set average=sum and dvmul=True to get an integrated value)

`pyspeckit.cubes.cubes.subimage_integ(cube, xcen, xwidth, ycen, ywidth, vrange, header=None, average=<function mean>, dvmult=False, return_HDU=False, units='pixels', zunits=None)`

Returns a sub-image from a data cube integrated over the specified velocity range

NOTE: With `spectral_cube`, subcube features can be easily applied with the `subcube` method, and integration is handled separately.

### Parameters

#### **cube**

[np.ndarray] A 3-dimensional numpy array with dimensions (velocity, y, x)

#### **xcen,ycen**

[float] The center in the X,Y-dimension. See `units` below for unit information

#### **xwidth,ywidth**

[float] The width in the X,Y-dimension. See `units` below for unit information xwidth and ywidth are “radius” values, i.e. half the length that will be extracted

#### **vrange**

[(float,float)] The velocity range to integrate over. See `zunits` below for unit information

**header**

[`astropy.io.fits.Header` or `None`] If specified, will allow the use of WCS units

**average**

[function] The function to apply when ‘integrating’ over the subcube

**dvmult**

[bool] If `dvmult` is set, multiply the average by DV (this is useful if you set `average=sum` and `dvmul=True` to get an integrated value, e.g. K km/s or Jy km/s)

**return\_hdu**

[bool] If specified, will return an HDU object, otherwise will return the array and header

**units**

[‘pixels’ or ‘wcs’] If ‘pixels’, all units (`xcen`, `ycen`, `xwidth`, `ywidth`) will be in pixels. If ‘wcs’, the values will be converted from WCS units to pixel units using the WCS specified by the header

**zunits**

[‘pixels’ or ‘wcs’ or `None`] If `None`, will be set to be the same as `units`

**Returns****subim, hdu**

[tuple] A tuple (integrated array, header) if `return_hdu` is `False`, or an HDU if it is `True`



## 6.1 Plain Text

Text files should be of the form:

```
wavelength flux err
3637.390 0.314 0.000
3638.227 0.717 0.000
3639.065 1.482 0.000
```

where there ‘err’ column is optional but the others are not. The most basic spectrum file allowed would have no header and two columns, e.g.:

```
1 0.5
2 1.5
3 0.1
```

If the X-axis is not monotonic, the data will be sorted so that the X-axis is in ascending order.

### 6.1.1 API

Routines for reading in ASCII format spectra. If atpy is not installed, will use a very simple routine for reading in the data.

```
pyspeckit.spectrum.readers.txt_reader.open_1d_txt(filename, xaxcol=0, datacol=1, errorcol=2,
                                                    text_reader='simple', format=None, **kwargs)
```

Attempt to read a 1D spectrum from a text file assuming wavelength as the first column, data as the second, and (optionally) error as the third.

Reading can be done either with `astropy.io.ascii` or a ‘simple’ reader. If you have an IPAC, CDS, or formally formatted table, you’ll want to use `astropy.io.ascii` and specify a format.

If you have a simply formatted file of the form, e.g. # name name # unit unit data data data data

kwargs are passed to `astropy.io.ascii.read`

```
pyspeckit.spectrum.readers.txt_reader.simple_txt(filename, xaxcol=0, datacol=1, errorcol=2,  
                                                  skiplines=0, **kwargs)
```

Very simple method for reading columns from ASCII file.

## 6.2 FITS

A minimal header should look like this:

```
SIMPLE =          T / conforms to FITS standard  
BITPIX =         -32 / array data type  
NAXIS  =          2 / number of array dimensions  
NAXIS1 =         659  
NAXIS2 =          2  
CRPIX1 =          1.0  
CRVAL1 = -4953.029632560421  
CDELTA1 = 212.5358581542998  
CTYPE1 = 'VRAD-LSR'  
CUNIT1 = 'm/s'  
BUNIT  = 'K'  
RESTFRQ = 110.20137E9  
SPECSYS = 'LSRK'  
END
```

A fits file with a header as above should be easily readable without any user effort:

```
sp = pyspeckit.Spectrum('test.fits')
```

If you have multiple spectroscopic axes, e.g.

```
CRPIX1A =          1.0  
CRVAL1A = 110.2031747948101  
CTYPE1A = 'FREQ-LSR'  
CUNIT1A = 'GHz'  
RESTFRQA= 110.20137
```

you can load that axis with the ‘wcstype’ keyword:

```
sp = pyspeckit.Spectrum('test.fits', wcstype='A')
```

If you have a .fits file with a non-linear X-axis that is stored in the .fits file as data (as opposed to being implicitly included in a header), you can load it using a custom .fits reader. An example implementation is given in the [tspec\\_reader](#). It can be registered using [Registration](#):

```
tspec_reader = check_reader(tspec_reader.tspec_reader)  
pyspeckit.register_reader('tspec', tspec_reader, 'fits')
```

### 6.2.1 API

```
pyspeckit.spectrum.readers.fits_reader.open_1d_fits(filename, hdu=0, **kwargs)
```

Grabs all the relevant pieces of a simple FITS-compliant 1d spectrum

**Inputs:**

**wcstype** - the suffix on the WCS type to get to  
velocity/frequency/whatever

**specnum** - Which # spectrum, along the y-axis, is  
the data?

**errspecnum** - Which # spectrum, along the y-axis,  
is the error spectrum?

```
pyspeckit.spectrum.readers.fits_reader.open_1d_pyfits(pyfits_hdu, specnum=0, wcstype="",
specaxis='1', errspecnum=None,
autofix=True, scale_keyword=None,
scale_action=<built-in function truediv>,
verbose=False, apnum=0, **kwargs)
```

This is open\_1d\_fits but for a pyfits\_hdu so you don't necessarily have to open a fits file

```
pyspeckit.spectrum.readers.fits_reader.read_echelle(pyfits_hdu)
```

Read an IRAF Echelle spectrum

<http://iraf.noao.edu/iraf/ftp/iraf/docs/specwcs.ps.Z>

## 6.3 hdf5

(work in progress)

### 6.3.1 API

Routines for reading in spectra from HDF5 files.

Note: Current no routines for parsing HDF5 headers in classes.py.

```
pyspeckit.spectrum.readers.hdf5_reader.open_hdf5(filename, xaxkey='xarr', datakey='data', er-
rkey='error')
```

This reader expects three datasets to exist in the hdf5 file 'filename': 'xarr', 'data', and 'error', by default. Can specify other dataset names.

## 6.4 Gildas CLASS files

Pyspeckit is capable of reading files from some versions of CLASS. The CLASS developers have stated that the GILDAS file format is private and will remain so, and therefore there are no guarantees that the CLASS reader will work for your file.

Nonetheless, if you want to develop in python instead of SIC, the `read_class` module is probably the best way to access CLASS data.

The `CLASS file specification` is incomplete, so much of the data reading is hacked together. The code style is based off of Tom Robitaille's `idlsave` package.

An example usage. Note that telescope and line are NOT optional keyword arguments, they are just specified as such for clarity

```
n2hp = class_to_obsblocks(fn1, telescope=['SMT-F1M-HU', 'SMT-F1M-VU'],
line=['N2HP(3-2)', 'N2H+(3-2)'])
```

This will generate a ObsBlock from all data tagged with the 'telescope' flags listed and lines matching either of those above. The data selection is equivalent to a combination of

```
find /telescope SMT-F1M-HU
find /telescope SMT-F1M-VU
find /line N2HP(3-2)
find /line N2H+(3-2)
```

ALL of the data matching those criteria will be included in an ObsBlock. They will then be accessible through the ObsBlock's `speclist` attribute, or just by indexing the ObsBlock directly.

## 6.4.1 An essentially undocumented API

### GILDAS CLASS file reader

Read a CLASS file into an `pyspeckit.spectrum.ObsBlock`

**class** `pyspeckit.spectrum.readers.read_class.LazyItem(parent)`  
Simple lazy spectrum-retriever wrapper

`pyspeckit.spectrum.readers.read_class.class_to_obsblocks(*arg, **kwargs)`  
Load an entire CLASS observing session into a list of ObsBlocks based on matches to the 'telescope', 'line' and 'source' names

#### Parameters

- filename**  
[string] The Gildas CLASS data file to read the spectra from.
- telescope**  
[list] List of telescope names to be matched.
- line**  
[list] List of line names to be matched.
- source**  
[list (optional)] List of source names to be matched. Defaults to None.
- imagfreq**  
[bool] Create a SpectroscopicAxis with the image frequency.

`pyspeckit.spectrum.readers.read_class.class_to_spectra(*arg, **kwargs)`  
Load each individual spectrum within a CLASS file into a list of Spectrum objects

`pyspeckit.spectrum.readers.read_class.downsample_1d(myarr, factor, estimator=<function mean>, weight=None)`  
Downsample a 1D array by averaging over *factor* pixels. Crops right side if the shape is not a multiple of factor.  
This code is pure numpy and should be fast.

#### keywords:

**estimator - default to mean. You can downsample by summing or**  
something else if you want a different estimator (e.g., downsampling error: you want to sum & divide by  $\sqrt{n}$ )

**weight: np.ndarray**  
An array of weights to use for the downsampling. If None, assumes uniform 1

`pyspeckit.spectrum.readers.read_class.ensure_bytes(string)`  
Ensure a given string is in byte form



pyspeckit.spectrum.readers.read\_class.filedescv2\_nw1 = 14

## GENERAL

integer(kind=obsnum\_length) :: num ! [ ] Observation number integer(kind=4) :: ver ! [ ] Version number  
integer(kind=4) :: teles(3) ! [ ] Telescope name integer(kind=4) :: dobs ! [MJD-60549] Date of observation  
integer(kind=4) :: dred ! [MJD-60549] Date of reduction integer(kind=4) :: typec ! [ code] Type of  
coordinates integer(kind=4) :: kind ! [ code] Type of data integer(kind=4) :: qual ! [ code] Quality of data  
integer(kind=4) :: subscan ! [ ] Subscan number integer(kind=obsnum\_length) :: scan ! [ ] Scan number !  
Written in the entry real(kind=8) :: ut ! 1-2 [ rad] UT of observation real(kind=8) :: st ! 3-4 [ rad] LST of  
observation real(kind=4) :: az ! 5 [ rad] Azimuth real(kind=4) :: el ! 6 [ rad] Elevation real(kind=4) :: tau !  
7 [neper] Opacity real(kind=4) :: tsys ! 8 [ K] System temperature real(kind=4) :: time ! 9 [ s] Integration  
time ! Not in this section in file integer(kind=4) :: xunit ! [ code] X unit (if X coordinates section is  
present) ! NOT in data — character(len=12) :: cdobs ! [string] Duplicate of dobs character(len=12) ::  
cdred ! [string] Duplicate of dred

pyspeckit.spectrum.readers.read\_class.gi8\_dicho(*ninp, lexn, xval, ceil=True*)

! @ public ! Find ival such as ! X(ival-1) < xval <= X(ival) (ceiling mode) ! or ! X(ival)  
<= xval < X(ival+1) (floor mode) ! for input data ordered. Use a dichotomic search for that. call  
gi8\_dicho(nex,file%desc%lexn,entry\_num,true,.,kex,error)

pyspeckit.spectrum.readers.read\_class.is\_ascii(*s*)

Check if there are non-ascii characters in Unicode string

### Parameters

*s*

[str] The string to be checked

### Returns

**is\_ascii**

[bool] Returns True if all characters in the string are ascii. False otherwise.

pyspeckit.spectrum.readers.read\_class.make\_axis(*header, imagfreq=False*)

Create a `pyspeckit.spectrum.units.SpectroscopicAxis` from the CLASS “header”

pyspeckit.spectrum.readers.read\_class.print\_timing(*func*)

Prints execution time of decorated function. Included here because CLASS files can take a little while to read;  
this should probably be replaced with a progressbar

pyspeckit.spectrum.readers.read\_class.read\_class(*\*arg, \*\*kwargs*)

Read a binary class file. Based on the [GILDAS CLASS file type Specification](#)

### Parameters

**filename:** str

**downsample\_factor:** None or int

Factor by which to downsample data by averaging. Useful for overresolved data.

**sourcename:** str or list of str

Source names to match to the data (uses regex)

**telescope:** str or list of str

‘XTEL’ or ‘TELE’ parameters: the telescope & instrument

**line: str or list of str**

The line name

**posang: tuple of 2 floats**

The first float is the minimum value for the position angle. The second float is the maximum value for the position angle.

**verbose: bool**

Log messages with severity INFO

**flag\_array: np.ndarray**

An array with the same shape as the data used to flag out (remove) data when downsampling.  
True = flag out

`pyspeckit.spectrum.readers.read_class.tests()`

Tests are specific to the machine on which this code was developed.

## 6.5 GBTIDL FITS files

GBTIDL SDFITS sessions can be loaded as `pyspeckit.ObsBlock` objects using the `GBTSession` reader:

```
gbtsession = pyspeckit.readers.GBTSession('AGBTsession.fits')
```

### 6.5.1 API

#### GBTIDL SDFITS file

GBTIDL SDFITS files representing GBT observing sessions can be read into `pyspeckit`. Additional documentation is needed. Nodding reduction is supported, frequency switching is not.

**class** `pyspeckit.spectrum.readers.gbt.GBTSession(sdfitsfile)`

A class wrapping all of the above features

Load an SDFITS file or a pre-loaded FITS file

**load\_target(*target*, *\*\*kwargs*)**

Load a Target...

**reduce\_all()**

**reduce\_target(*target*, *\*\*kwargs*)**

Reduce the data for a given object name

**class** `pyspeckit.spectrum.readers.gbt.GBTTarget(Session, target, **kwargs)`

A collection of `ObsBlocks` or `Spectra`

Container for the individual scans of a target from a GBT session

**reduce(*obstype*='nod', *\*\*kwargs*)**

Reduce noddred observations (they should have been read in `__init__`)

`pyspeckit.spectrum.readers.gbt.average_IF(block, debug=False)`

Average the polarizations for each feed in each IF

`pyspeckit.spectrum.readers.gbt.average_pols(block)`

Average the polarizations for each feed in each IF

`pyspeckit.spectrum.readers.gbt.count_integrations(sdfitsfile, target)`  
 Return the number of integrations for a given target (uses one sampler; assumes same number for all samplers)

`pyspeckit.spectrum.readers.gbt.dcmeantsys(calon, caloff, tcal, debug=False)`  
 from GBTIDL's `dcmeantsys.py` ;  $\text{mean\_tsys} = \text{tcal} * \text{mean}(\text{nocal}) / (\text{mean}(\text{withcal} - \text{nocal})) + \text{tcal}/2.0$

`pyspeckit.spectrum.readers.gbt.find_feeds(block)`  
 Get a dictionary of the feed numbers for each sampler

`pyspeckit.spectrum.readers.gbt.find_matched_freqs(reduced_blocks, debug=False)`  
 Use frequency-matching to find which samplers observed the same parts of the spectrum

**WARNING** These IF numbers don't match GBTIDL's! I don't know how to get those to match up!

`pyspeckit.spectrum.readers.gbt.find_pols(block)`  
 Get a dictionary of the polarization for each sampler

`pyspeckit.spectrum.readers.gbt.identify_samplers(block)`  
 Identify each sampler with an IF number, a feed number, and a polarization

`pyspeckit.spectrum.readers.gbt.list_targets(sdfitsfile, doprint=True)`  
 List the targets, their location on the sky...

`pyspeckit.spectrum.readers.gbt.read_gbt_scan(sdfitsfile, obsnumber=0)`  
 Read a single scan from a GBTIDL SDFITS file

`pyspeckit.spectrum.readers.gbt.read_gbt_target(sdfitsfile, objectname, verbose=False)`  
 Give an object name, get all observations of that object as an 'obsblock'

`pyspeckit.spectrum.readers.gbt.reduce_gbt_target(sdfitsfile, objectname, nbeams, verbose=False)`  
 Wrapper - read an SDFITS file, get an object, reduce it (assuming noddod) and return it

`pyspeckit.spectrum.readers.gbt.reduce_nod(blocks, verbose=False, average=True, fdid=(1, 2))`  
 Do a noddod on/off observation given a dict of observation blocks as produced by `read_gbt_target`

#### Parameters

**fdid**

[2-tuple]

`pyspeckit.spectrum.readers.gbt.reduce_totalpower(blocks, verbose=False, average=True, fdid=1)`  
 Reduce a total power observation

`pyspeckit.spectrum.readers.gbt.round_to_resolution(frequency, resolution)`  
 kind of a hack, but round the frequency to the nearest integer multiple of the resolution, then multiply it back into frequency space

`pyspeckit.spectrum.readers.gbt.sigref(nod1, nod2, tsys_nod2)`  
 Signal-Reference ('nod') calibration ;  $((\text{dcsig} - \text{dcres}) / \text{dcres}) * \text{dcres} \cdot \text{tsys}$  see GBTIDL's `dosigref`

`pyspeckit.spectrum.readers.gbt.totalpower(calon, caloff, average=True)`  
 Do a total-power calibration of an on/off data set (see `dototalpower.pro` in GBTIDL)

`pyspeckit.spectrum.readers.gbt.uniq(seq)`  
 from <http://stackoverflow.com/questions/480214/how-do-you-remove-duplicates-from-a-list-in-python-whilst-preserving-order>



These are wrappers to simplify some of the more complicated (and even some of the simpler) functions in PySpecKit

## 7.1 Cube Fitting

Complicated code for fitting of a whole data cube, pixel-by-pixel

```
pyspeckit.wrappers.cube_fit.cube_fit(cubefilename, outfilename, errfilename=None,
                                     scale_keyword=None, vheight=False, verbose=False, signal_cut=3, verbose_level=2, overwrite=True, **kwargs)
```

Light-weight wrapper for cube fitting

Takes a cube and error map (error will be computed naively if not given) and computes moments then fits for each spectrum in the cube. It then saves the fitted parameters to a reasonably descriptive output file whose header will look like

```
PLANE1 = 'amplitude'
PLANE2 = 'velocity'
PLANE3 = 'sigma'
PLANE4 = 'err_amplitude'
PLANE5 = 'err_velocity'
PLANE6 = 'err_sigma'
PLANE7 = 'integral'
PLANE8 = 'integral_error'
CDEL3 = 1
CTYPE3 = 'FITPAR'
CRVAL3 = 0
CRPIX3 = 1
```

### Parameters

**errfilename:** [ None | string name of .fits file ]

A two-dimensional error map to use for computing signal-to-noise cuts

**scale\_keyword:** [ None | Char ]

Keyword to pass to the data cube loader - multiplies cube by the number indexed by this header kwarg if it exists. e.g., if your cube is in T\_A units and you want T\_A\*

**vheight:** [ bool ]

Is there a background to be fit? Used in moment computation

**verbose:** [ bool ]

**verbose\_level:** [ int ]

How loud will the fitting procedure be? Passed to momenteach and fiteach

**signal\_cut:** [ float ]

Signal-to-Noise ratio minimum. Spectra with a peak below this S/N ratio will not be fit and will be left blank in the output fit parameter cube

**overwrite:** [ bool ]

Overwrite parameter .fits cube if it exists?

**‘kwargs’ are passed to :class:‘pyspeckit.Spectrum.specfit‘**

```
pyspeckit.wrappers.fit_gaussians_to_simple_spectra.fit_gaussians_to_simple_spectra(filename,  
unit='km/s',  
do-  
plot=True,  
base-  
line=True,  
plotresid-  
u-  
als=False,  
figure-  
save-  
name=None,  
cro-  
prange=None,  
save-  
name=None,  
**kwargs)
```

As stated in the name title, will fit Gaussians to simple spectra!

kwargs will be passed to specfit

**figuresave** [ None | string ]

After fitting, save the figure to this filename if specified

**crop** [ list of 2 floats ]

Crop the spectrum to (min,max) in the specified units

**save** [ None | string ]

After fitting, save the spectrum to this filename

Note that this wrapper can be used from the command line:

```
python fit_gaussians_to_simple_spectra.py spectrum.fits
```

## 7.2 NH3 fitter wrapper

Wrapper to fit ammonia spectra. Generates a reasonable guess at the position and velocity using a gaussian fit

Example use:

```
import pyspeckit
sp11 = pyspeckit.Spectrum('spec.nh3_11.dat', errorcol=999)
sp22 = pyspeckit.Spectrum('spec.nh3_22.dat', errorcol=999)
sp33 = pyspeckit.Spectrum('spec.nh3_33.dat', errorcol=999)
sp11.xarr.refX = pyspeckit.spectrum.models.ammonia.freq_dict['oneone']
sp22.xarr.refX = pyspeckit.spectrum.models.ammonia.freq_dict['twotwo']
sp33.xarr.refX = pyspeckit.spectrum.models.ammonia.freq_dict['threethree']
input_dict={'oneone':sp11, 'twotwo':sp22, 'threethree':sp33}
spf = pyspeckit.wrappers.fitnh3.fitnh3tkin(input_dict)
```

`pyspeckit.wrappers.fitnh3.BigSpectrum_to_NH3dict(sp, vrange=None)`

A rather complicated way to make the spdicts above given a spectrum...

`pyspeckit.wrappers.fitnh3.fitnh3(spectrum, vrange=[-100, 100], vrangeunit='km/s', quiet=False, Tex=20, trot=15, column=1000000000000000.0, fortho=1.0, tau=None, Tkin=None, spec_convert_kwargs={})`

`pyspeckit.wrappers.fitnh3.fitnh3tkin(input_dict, dobaseline=True, baselinekwargs={}, crop=False, cropunit=None, guessline='twotwo', tex=15, trot=20, column=15.0, fortho=0.66, tau=None, thin=False, quiet=False, doplot=True, fignum=1, guessfignum=2, smooth=False, scale_keyword=None, rebase=False, tkin=None, npeaks=1, guesses=None, guess_error=True, plotter_wrapper_kwargs={}, **kwargs)`

Given a dictionary of filenames and lines, fit them together e.g. {'oneone': 'G000.000+00.000\_nh3\_11.fits'}

### Parameters

#### **input\_dict**

[dict] A dictionary in which the keys are the ammonia line names (e.g., 'oneone', 'twotwo', etc) and the values are either Spectrum objects or filenames of spectra

#### **dobaseline**

[bool] Fit and subtract a baseline prior to fitting the model? Keyword arguments to `pyspeckit.spectrum.Spectrum.baseline` are specified in `baselinekwargs`.

#### **baselinekwargs**

[dict] The keyword arguments for the baseline

#### **crop**

[bool or tuple] A range of values to crop the spectrum to. The units are specified by `cropunit`; the default None will use pixels. If False, no cropping will be performed.

#### **cropunit**

[None or astropy unit] The unit for the crop parameter

#### **guess\_error**

[bool] Use the guess line to estimate the error in all spectra?

#### **plotter\_wrapper\_kwargs**

[dict] Keyword arguments to pass to the plotter

pyspeckit.wrappers.fitnh3.**make\_axdict**(*splist*, *spdict*)

pyspeckit.wrappers.fitnh3.**plot\_nh3**(*spdict*, *spectra*, *fignum*=1, *show\_components*=False, *resid\_fignum*=None, *show\_hyperfine\_components*=True, *annotate*=True, *axdict*=None, *figure*=None, *\*\*plotkwargs*)

Plot the results from a multi-nh3 fit

**spdict needs to be dictionary with form:**

‘oneone’: spectrum, ‘twotwo’: spectrum, etc.

pyspeckit.wrappers.fitnh3.**plotter\_override**(*sp*, *vrange*=None, *\*\*kwargs*)

Do plot\_nh3 with syntax similar to plotter()

## 7.3 N2H+ fitter wrapper

Wrapper to fit N2H+ using RADEX models. This is meant to be used from the command line, e.g.

```
python n2hp_wrapper.py file.fits
```

and therefore has no independently defined functions.

pyspeckit.wrappers.n2hp\_wrapper.**make\_n2hp\_fitter**(*path\_to\_radex*='/Users/adam/work/n2hp/',  
*fileprefix*='1-2\_T=5to55\_lvg')

Create a n2hp fitter using RADEX data cubes. The following files must exist:

```
path_to_radex+fileprefix+'_tex1.fits'  
path_to_radex+fileprefix+'_tau1.fits'  
path_to_radex+fileprefix+'_tex2.fits'  
path_to_radex+fileprefix+'_tau2.fits'
```

e.g. /Users/adam/work/n2hp/1-2\_T=5to55\_lvg\_tau1.fits

## 7.4 N2H+ extras

In place of the actual contents of N2H+ fitter, here are the modules used to make the wrapper

```
class pyspeckit.spectrum.models.model.SpectralModel(modelfunc, npars, shortvarnames=('A',  
                                         '\Delta x', '\sigma'), fitunit=None, centroid_par=None,  
                                         fwhm_func=None, fwhm_pars=None, integral_func=None,  
                                         use_lmfit=False, guess_types=('amplitude',  
                                         'center', 'width'), **kwargs)
```

A wrapper class for a spectra model. Includes internal functions to generate multi-component models, annotations, integrals, and individual components. The declaration can be complex, since you should name individual variables, set limits on them, set the units the fit will be performed in, and set the annotations to be used. Check out some of the hyperfine codes (hcn, n2hp) for examples.

Spectral Model Initialization

Create a Spectral Model class for data fitting

**Parameters**



**modelfunc**

[function] the model function to be fitted. Should take an X-axis (spectroscopic axis) as an input followed by input parameters. Returns an array with the same shape as the input X-axis

**npars**

[int] number of parameters required by the model

**parnames**

[list (optional)] a list or tuple of the parameter names

**parvalues**

[list (optional)] the initial guesses for the input parameters (defaults to ZEROS)

**parlimits**

[list (optional)] the upper/lower limits for each variable (defaults to ZEROS)

**parfixed**

[list (optional)] Can declare any variables to be fixed (defaults to ZEROS)

**parerror**

[list (optional)] technically an output parameter. Specifying it here will have no effect. (defaults to ZEROS)

**partied**

[list (optional)] not the past tense of party. Can declare, via text, that some parameters are tied to each other. Defaults to zeros like the others, but it's not clear if that's a sensible default

**fitunit**

[str (optional)] convert X-axis to these units before passing to model

**parsteps**

[list (optional)] minimum step size for each parameter (defaults to ZEROS)

**npeaks**

[list (optional)] default number of peaks to assume when fitting (can be overridden)

**shortvarnames**

[list (optional)] TeX names of the variables to use when annotating

**amplitude\_types**

[tuple] A tuple listing the types of the different parameters when guessing. The valid values are 'amplitude', 'width', and 'center'. These are handled by `parse_3par_guesses`, which translate these into input guess lists for the fitter. For a "standard" 3-parameter Gaussian fitter, nothing changes, but for other models that have more than 3 parameters, some translation is needed.

**Returns**

**A tuple containing (model best-fit parameters, the model, parameter**

**errors,  $\chi^2$  value)**

```
n2hp.n2hp_radex(density=4, column=13, xoff_v=0.0, width=1.0, grid_vwidth=1.0,
                grid_vwidth_scale=False, texgrid=None, taugrid=None, hdr=None, path_to_texgrid="",
                path_to_taugrid="", temperature_gridnumber=3, debug=False, verbose=False, **kwargs)
```

Use a grid of RADEX-computed models to make a model line spectrum

The RADEX models have to be available somewhere. OR they can be passed as arrays. If as arrays, the form should be: `texgrid = ((minfreq1,maxfreq1,texgrid1),(minfreq2,maxfreq2,texgrid2))`

`xarr` must be a `SpectroscopicAxis` instance `xoff_v`, `width` are both in km/s

`grid_vwidth` is the velocity assumed when computing the grid in km/s this is important because  $\tau = \text{modeltau} / \text{width}$  (see, e.g., Draine 2011 textbook pgs 219-230) `grid_vwidth_scale` is True or False: False for LVG, True for Sphere

Check out the [flickr gallery](#).

Want your image or example included? [E-mail us](#).

## 8.1 Creating a Spectrum from scratch

This example shows the initialization of a pyspeckit object from numpy arrays.

```
import numpy as np
import pyspeckit

xaxis = np.linspace(-50,150,100.)
sigma = 10.
center = 50.
synth_data = np.exp(-(xaxis-center)**2/(sigma**2 * 2.))

# Add noise
stddev = 0.1
noise = np.random.randn(xaxis.size)*stddev
error = stddev*np.ones_like(synth_data)
data = noise+synth_data

# this will give a "blank header" warning, which is fine
sp = pyspeckit.Spectrum(data=data, error=error, xarr=xaxis,
                        xarrkwargs={'unit': 'km/s'},
                        unit='erg/s/cm^2/AA')

sp.plotter()

# Fit with automatic guesses
sp.specfit(fittype='gaussian')
```

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```
# Fit with input guesses
# The guesses initialize the fitter
# This approach uses the 0th, 1st, and 2nd moments
amplitude_guess = data.max()
center_guess = (data*xaxis).sum()/data.sum()
width_guess = (data.sum() / amplitude_guess / (2*np.pi))**0.5
guesses = [amplitude_guess, center_guess, width_guess]
sp.specfit(fittype='gaussian', guesses=guesses)

sp.plotter(errstyle='fill')
sp.specfit.plot_fit()
```

## 8.2 Fitting a continuum model as a model

This example shows the initialization of a pyspeckit object from numpy arrays, as in *Creating a Spectrum from scratch*, but it adds the twist of including a steep continuum.

We fit the continuum using the polynomial continuum model, which gives access to the error on the polynomial fit parameters. No such parameters are accessible via the `pyspeckit.Spectrum.baseline` tools because they use `numpy.poly1d` to fit the data.

```
import numpy as np
import pyspeckit

xaxis = np.linspace(-50,150,100.)
sigma = 10.
center = 50.

baseline = np.poly1d([0.1, 0.25])(xaxis)

synth_data = np.exp(-(xaxis-center)**2/(sigma**2 * 2.)) + baseline

# Add noise
stddev = 0.1
noise = np.random.randn(xaxis.size)*stddev
error = stddev*np.ones_like(synth_data)
data = noise+synth_data

# this will give a "blank header" warning, which is fine
sp = pyspeckit.Spectrum(data=data, error=error, xarr=xaxis,
                        xarrkwargs={'unit': 'km/s'},
                        unit='erg/s/cm^2/AA')

sp.plotter()

sp.specfit.Registry.add_fitter('polycontinuum',
                               pyspeckit.models.polynomial_continuum.poly_fitter(),
                               2)

sp.specfit(fittype='polycontinuum', guesses=(0,0), exclude=[30, 70])

# subtract the model fit to create a new spectrum
sp_contsub = sp.copy()
sp_contsub.data -= sp.specfit.get_full_model()
```

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```

sp_contsub.plotter()

# Fit with automatic guesses
sp_contsub.specfit(fittype='gaussian')

# Fit with input guesses
# The guesses initialize the fitter
# This approach uses the 0th, 1st, and 2nd moments
data = sp_contsub.data
amplitude_guess = data.max()
center_guess = (data*xaxis).sum()/data.sum()
width_guess = (data.sum() / amplitude_guess / (2*np.pi))**0.5
guesses = [amplitude_guess, center_guess, width_guess]
sp_contsub.specfit(fittype='gaussian', guesses=guesses)

sp_contsub.plotter(errstyle='fill')
sp_contsub.specfit.plot_fit()

```

## 8.3 Cube Fitting: a lightweight gaussian example

```

import pyspeckit
from pyspeckit.cubes.tests.test_cubetools import make_test_cube
import matplotlib.pyplot as plt
import numpy as np

# generate a test spectral cube (10x10, with a 100 spectral channels)
make_test_cube((100,10,10), outfile='test.fits')
spc = pyspeckit.Cube('test.fits')

# do a crude noise estimate on the 30 edge channels
rmsmap = np.vstack([spc.cube[:15], spc.cube[85:]]).std(axis=0)

# get a cube of moments
spc.momenteach(vheight=False)

# fit each pixel taking its moment as an initial guess
spc.fiteach(fittype = 'gaussian',
            guesses = spc.momentcube,
            errmap = rmsmap,
            signal_cut = 3, # ignore pixels with SNR<3
            blank_value = np.nan,
            start_from_point=(5,5))
spc.mapplot()
# show the fitted amplitude
spc.show_fit_param(0, cmap='viridis')
plt.show()

```

## 8.4 Cube Fitting: simple, from scratch example

```

"""
simple cube fitting example

```

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```

"""
from __future__ import print_function

import numpy as np
import pyspeckit
from spectral_cube import SpectralCube
from astropy import wcs
from astropy import units as u

# Create a new WCS object so we can instantiate the SpectralCube
mywcs = wcs.WCS(naxis=3)

# Set up a tangent projection
# You would normally read this from a file!!
mywcs.wcs.crpix = [1,2,21.0]
mywcs.wcs.cdelt = np.array([-0.066667, 0.066667, 500])
mywcs.wcs.crval = [290.9250, 14.5092, 60000]
mywcs.wcs.ctype = ["RA---TAN", "DEC--TAN", 'VELO']
mywcs.wcs.cunit = ['deg', 'deg', 'm/s']

# Create a synthetic X-dimension in km/s
xarr = np.linspace(50, 70, 41) # km/s

# Define a line width, which will vary across our image
# It will increase from 1 km/s to 4 km/s over the X-direction (RA)
sigma = np.outer(np.linspace(1,1.5,2), np.ones(4)).T

# Define a line center, which will vary in the opposite direction,
# along increasing Y-direction (declination)
centroid = np.outer(np.ones(2), np.linspace(58, 62, 4)).T

data = np.exp(-(np.tile(xarr, (2, 4, 1)).T - centroid)**2 / (2.*sigma**2))
cube = SpectralCube(data=data, wcs=mywcs)

# Sanity checks: do the moments accurately recover the inputs?
assert (np.abs(cube.moment1().to(u.km/u.s).value - centroid).max()) < 1e-5
assert (np.abs(cube.moment2().to(u.km**2/u.s**2).value - sigma**2).max()) < 1e-5

# Create a pyspeckit cube
pcube = pyspeckit.Cube(cube=cube)

# For convenience, convert the X-axis to km/s
# (WCSLIB automatically converts to m/s even if you give it km/s)
pcube.xarr.convert_to_unit(u.km/u.s)

# Set up the fitter by doing a preliminary fit
pcube.specfit(fittype='gaussian', guesses='moments')

# Fit each spectrum with a gaussian
# First, assemble the guesses:
guesses = np.array([cube.max(axis=0).value,
                    cube.moment1(axis=0).to(u.km/u.s).value,
                    (cube.moment2(axis=0)**0.5).to(u.km/u.s).value])
# (the second moment is in m^2/s^2, but we want km/s

# Do the fit!
pcube.fiteach(guesses=guesses, # pass in the guess array

```

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```

        # tell it where to start the fitting (center pixel in this case)
        start_from_point=(5,5),
        # Paralellize the fits?
        multicore=4,
        fittype='gaussian',
    )

# Then you can access the fits via parcube:
assert np.all(pcube.parcube[0,:,:] == 1)
assert np.all(pcube.parcube[1,:,:] == centroid)
assert np.all(pcube.parcube[2,:,:] == sigma)

# Can also fit non-parallelized
pcube.fiteach(guesses=guesses, # pass in the guess array
              # tell it where to start the fitting (center pixel in this case)
              start_from_point=(5,5),
              # Paralellize the fits?
              multicore=1,
              fittype='gaussian',
              )

assert np.all(pcube.parcube[0,:,:] == 1)
assert np.all(pcube.parcube[1,:,:] == centroid)
assert np.all(pcube.parcube[2,:,:] == sigma)

```

## 8.5 Radio Fitting: H<sub>2</sub>CO RADEX example

Because an LVG model grid is being used as the basis for the fitting in this example, there are fewer free parameters. If you want to create your own model grid, there is a set of tools for creating RADEX model grids (in parallel) at the [agpy RADEX page](#). The model grids used below are available on the [pyspeckit bitbucket download page](#).

```

import pyspeckit
import numpy as np
import pyfits
from pyspeckit.spectrum import models

# create the Formaldehyde Radex fitter
# This step cannot be easily generalized: the user needs to read in their own grids
texgrid1 = pyfits.getdata('/Users/adam/work/h2co/radex/grid_greenscaled/1-1_2-2_T5to55_lvg_greenscaled_
↳ tex1.fits')
taugrid1 = pyfits.getdata('/Users/adam/work/h2co/radex/grid_greenscaled/1-1_2-2_T5to55_lvg_greenscaled_
↳ tau1.fits')
texgrid2 = pyfits.getdata('/Users/adam/work/h2co/radex/grid_greenscaled/1-1_2-2_T5to55_lvg_greenscaled_
↳ tex2.fits')
taugrid2 = pyfits.getdata('/Users/adam/work/h2co/radex/grid_greenscaled/1-1_2-2_T5to55_lvg_greenscaled_
↳ tau2.fits')
hdr = pyfits.getheader('/Users/adam/work/h2co/radex/grid_greenscaled/1-1_2-2_T5to55_lvg_greenscaled_
↳ tau2.fits')

# this deserves a lot of explanation:
# models.formaldehyde_radex is the MODEL that we are going to fit
# models.model.SpectralModel is a wrapper to deal with parinfo, multiple peaks,
# and annotations
# all of the parameters after the first are passed to the model function

```

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```

formaldehyde_radex_fitter = models.model.SpectralModel(
    models.formaldehyde.formaldehyde_radex, 4,
    parnames=['density', 'column', 'center', 'width'],
    parvalues=[4,12,0,1],
    parlimited=[(True,True), (True,True), (False,False), (True,False)],
    parlimits=[(1,8), (11,16), (0,0), (0,0)],
    parsteps=[0.01,0.01,0,0],
    fitunits='Hz',
    texgrid=((4,5,texgrid1),(14,15,texgrid2)), # specify the frequency range over which the grid is_
    ↪valid (in GHz)
    taugrid=((4,5,taugrid1),(14,15,taugrid2)),
    hdr=hdr,
    shortvarnames=("n", "N", "v", "\\sigma"), # specify the parameter names (TeX is OK)
    grid_vwidth_scale=False,
)

# sphere version:
texgrid1 = pyfits.getdata('/Users/adam/work/h2co/radex/grid_aug2011_sphere/grid_aug2011_sphere_tex1.fits
    ↪')
taugrid1 = pyfits.getdata('/Users/adam/work/h2co/radex/grid_aug2011_sphere/grid_aug2011_sphere_tau1.fits
    ↪')
texgrid2 = pyfits.getdata('/Users/adam/work/h2co/radex/grid_aug2011_sphere/grid_aug2011_sphere_tex2.fits
    ↪')
taugrid2 = pyfits.getdata('/Users/adam/work/h2co/radex/grid_aug2011_sphere/grid_aug2011_sphere_tau2.fits
    ↪')
hdr = pyfits.getheader('/Users/adam/work/h2co/radex/grid_aug2011_sphere/grid_aug2011_sphere_tau2.fits')

formaldehyde_radex_fitter_sphere = models.model.SpectralModel(
    models.formaldehyde.formaldehyde_radex, 4,
    parnames=['density', 'column', 'center', 'width'],
    parvalues=[4,12,0,1],
    parlimited=[(True,True), (True,True), (False,False), (True,False)],
    parlimits=[(1,8), (11,16), (0,0), (0,0)],
    parsteps=[0.01,0.01,0,0],
    fitunits='Hz',
    texgrid=((4,5,texgrid1),(14,15,texgrid2)),
    taugrid=((4,5,taugrid1),(14,15,taugrid2)),
    hdr=hdr,
    shortvarnames=("n", "N", "v", "\\sigma"),
    grid_vwidth_scale=True,
)

sp1 = pyspeckit.Spectrum('G203.04+1.76_h2co.fits', wcstype='D', scale_keyword='ETAMB')
sp2 = pyspeckit.Spectrum('G203.04+1.76_h2co_Tastar.fits', wcstype='V', scale_keyword='ETAMB')

sp1.crop(-50,50)
sp1.smooth(3) # match to GBT resolution
sp2.crop(-50,50)

sp1.xarr.convert_to_unit('GHz')
sp1.specfit() # determine errors
sp1.error = np.ones(sp1.data.shape)*sp1.specfit.residuals.std()
sp1.baseline(excludefit=True)
sp2.xarr.convert_to_unit('GHz')

```

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```

sp2.specfit() # determine errors
sp2.error = np.ones(sp2.data.shape)*sp2.specfit.residuals.std()
sp2.baseline(excludefit=True)
sp = pyspeckit.Spectra([sp1,sp2])

sp.Registry.add_fitter('formaldehyde_radex',
    formaldehyde_radex_fitter,4)
sp.Registry.add_fitter('formaldehyde_radex_sphere',
    formaldehyde_radex_fitter_sphere,4)

sp.plotter()
sp.specfit(fittype='formaldehyde_radex',multifit=None,guesses=[4,12,3.75,0.43],quiet=False)

# these are just for pretty plotting:
sp1.specfit.fitter = sp.specfit.fitter
sp1.specfit.modelpars = sp.specfit.modelpars
sp1.specfit.model = np.interp(sp1.xarr,sp.xarr,sp.specfit.model)
sp2.specfit.fitter = sp.specfit.fitter
sp2.specfit.modelpars = sp.specfit.modelpars
sp2.specfit.model = np.interp(sp2.xarr,sp.xarr,sp.specfit.model)

# previously, xarrs were in GHz to match the fitting scheme
sp1.xarr.convert_to_unit('km/s')
sp2.xarr.convert_to_unit('km/s')

sp1.plotter(xmin=-5,xmax=15,errstyle='fill')
sp1.specfit.plot_fit(show_components=True)
sp2.plotter(xmin=-5,xmax=15,errstyle='fill')
sp2.specfit.plot_fit(show_components=True)

sp.plotter(figure=5)
sp.specfit(fittype='formaldehyde_radex_sphere',multifit=None,guesses=[4,13,3.75,0.43],quiet=False)

# these are just for pretty plotting:
sp1.specfit.fitter = sp.specfit.fitter
sp1.specfit.modelpars = sp.specfit.modelpars
sp1.specfit.model = np.interp(sp1.xarr.as_unit('GHz'),sp.xarr,sp.specfit.model)
sp2.specfit.fitter = sp.specfit.fitter
sp2.specfit.modelpars = sp.specfit.modelpars
sp2.specfit.model = np.interp(sp2.xarr.as_unit('GHz'),sp.xarr,sp.specfit.model)

sp1.plotter(xmin=-5,xmax=15,errstyle='fill',figure=6)
sp1.specfit.plot_fit(show_components=True)
sp2.plotter(xmin=-5,xmax=15,errstyle='fill',figure=7)
sp2.specfit.plot_fit(show_components=True)

```

## 8.6 Radio Fitting: H<sub>2</sub>CO millimeter thermometer lines

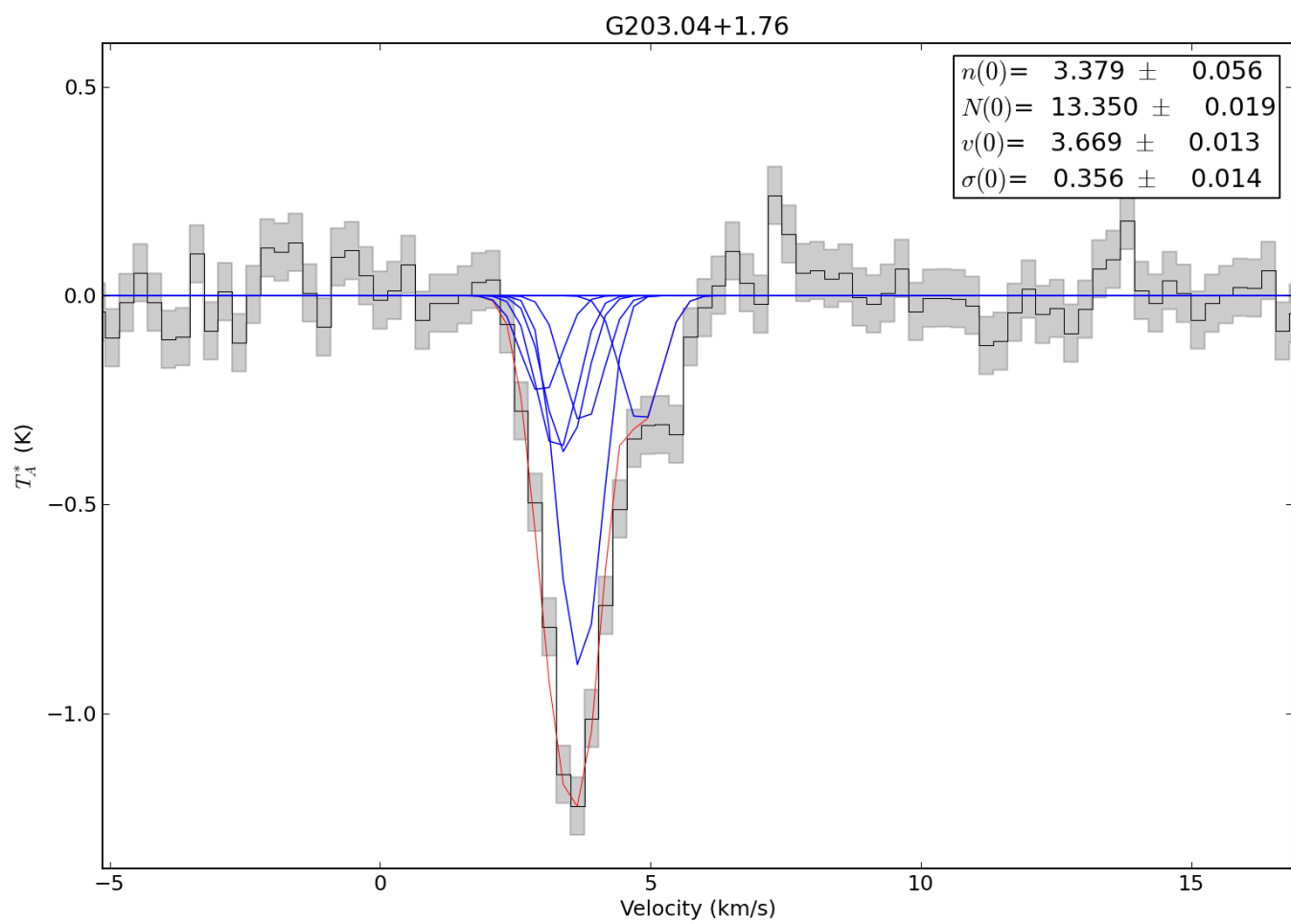
Example hyperfine line fitting of a data cube for the H<sub>2</sub>CO 303-202, 321-220, and 322-221 lines.

```

import pyspeckit
try:
    import astropy.io.fits as pyfits

```

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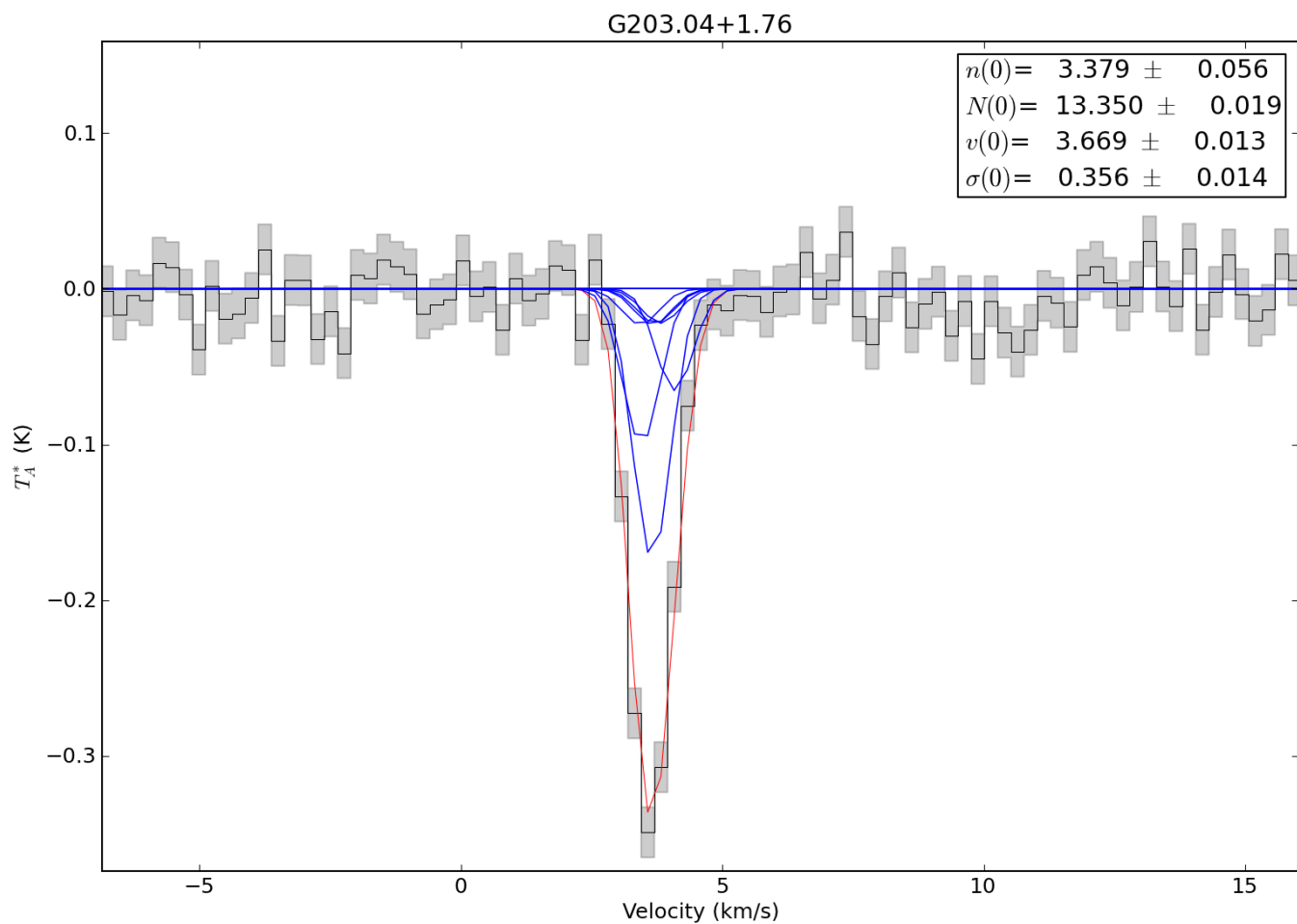


Fig. 1: Both transitions are fit simultaneously using a RADEX model. The input (fitted) parameters are therefore density, column density, width, and velocity.

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```

except ImportError:
    import pyfits
from pyspeckit.spectrum import models

# create the Formaldehyde Radex fitter
# This step cannot be easily generalized: the user needs to read in their own grids
# Some of these grids can be acquired from:
# https://github.com/keflavich/radex_data_grids
texgrid1 = pyfits.getdata('/Users/adam/work/h2co/radex/thermom/303-202_321-220_5kms_temperature_para_
↳tex1.fits')
taugrid1 = pyfits.getdata('/Users/adam/work/h2co/radex/thermom/303-202_321-220_5kms_temperature_para_
↳tau1.fits')
texgrid2 = pyfits.getdata('/Users/adam/work/h2co/radex/thermom/303-202_321-220_5kms_temperature_para_
↳tex2.fits')
taugrid2 = pyfits.getdata('/Users/adam/work/h2co/radex/thermom/303-202_321-220_5kms_temperature_para_
↳tau2.fits')
hdr = pyfits.getheader('/Users/adam/work/h2co/radex/thermom/303-202_321-220_5kms_temperature_para_tau2.
↳fits')

texgrid1b = pyfits.getdata('/Users/adam/work/h2co/radex/thermom/303-202_322-221_5kms_temperature_para_
↳tex1.fits')
taugrid1b = pyfits.getdata('/Users/adam/work/h2co/radex/thermom/303-202_322-221_5kms_temperature_para_
↳tau1.fits')
texgrid2b = pyfits.getdata('/Users/adam/work/h2co/radex/thermom/303-202_322-221_5kms_temperature_para_
↳tex2.fits')
taugrid2b = pyfits.getdata('/Users/adam/work/h2co/radex/thermom/303-202_322-221_5kms_temperature_para_
↳tau2.fits')
hdrb = pyfits.getheader('/Users/adam/work/h2co/radex/thermom/303-202_322-221_5kms_temperature_para_tau2.
↳fits')

# this deserves a lot of explanation:
# models.formaldehyde.formaldehyde_radex is the MODEL that we are going to fit
# models.model.SpectralModel is a wrapper to deal with parinfo, multiple peaks,
# and annotations
# all of the parameters after the first are passed to the model function
# This first one fits only the 303-202 and 322-221 lines
formaldehyde_radex_fitter_b = models.model.SpectralModel(
    models.formaldehyde_mm.formaldehyde_mm_radex, 5,
    parnames=['temperature', 'column', 'density', 'center', 'width'],
    parvalues=[50,12,4.5,0,1],
    parlimited=[(True,True), (True,True), (True,True), (False,False), (True,False)],
    parlimits=[(5,205), (10,17), (2,7), (0,0), (0,0)],
    parsteps=[0.01,0.01,0.1,0,0],
    fitunits='Hz',
    texgrid=((218.2,218.3,texgrid1b),(218.4,218.55,texgrid2b)), # specify the frequency range over_
↳which the grid is valid (in GHz)
    taugrid=((218.2,218.3,taugrid1b),(218.4,218.55,taugrid2b)),
    hdr=hdrb,
    shortvarnames=("T", "N", "n", "v", "\\sigma"), # specify the parameter names (TeX is OK)
    grid_vwidth=5.0,
)

# This second fitter fits only the 303-202 and 321-220 lines
formaldehyde_radex_fitter = models.model.SpectralModel(
    models.formaldehyde_mm.formaldehyde_mm_radex, 5,
    parnames=['temperature', 'column', 'density', 'center', 'width'],
    parvalues=[50,12,4.5,0,1],

```

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```

parlimited=[(True,True), (True,True), (True,True), (False,False), (True,False)],
parlimits=[(5,205), (10,17), (2,7), (0,0), (0,0)],
parsteps=[0.01,0.01,0.1,0,0],
fitunits='Hz',
texgrid=((218.2,218.3,texgrid1),(218.7,218.8,texgrid2)), # specify the frequency range over which
↳the grid is valid (in GHz)
taugrid=((218.2,218.3,taugrid1),(218.7,218.8,taugrid2)),
hdr=hdr,
shortvarnames=("T","N","n","v","\\sigma"), # specify the parameter names (TeX is OK)
grid_vwidth=5.0,
)

# This third fitter fits all three of the 303-202, 322-221, and 321-220 lines
# Since it has no additional free parameters, it's probably best...
formaldehyde_radex_fitter_both = models.model.SpectralModel(
    models.formaldehyde_mm.formaldehyde_mm_radex, 5,
    parnames=['temperature','column','density','center','width'],
    parvalues=[50,12,4.5,0,1],
    parlimited=[(True,True), (True,True), (True,True), (False,False), (True,False)],
    parlimits=[(5,205), (10,17), (2,7), (0,0), (0,0)],
    parsteps=[0.01,0.01,0.1,0,0],
    fitunits='Hz',
    texgrid=((218.2,218.3,texgrid1b),(218.4,218.55,texgrid2b),(218.7,218.8,texgrid2)), # specify the
↳frequency range over which the grid is valid (in GHz)
    taugrid=((218.2,218.3,taugrid1b),(218.4,218.55,taugrid2b),(218.7,218.8,taugrid2)),
    hdr=hdrb,
    shortvarnames=("T","N","n","v","\\sigma"), # specify the parameter names (TeX is OK)
    grid_vwidth=5.0,
)

if __name__ == "__main__":

    import pyspeckit.spectrum.readers.read_class
    sp = pyspeckit.readers.read_class.class_to_spectra('example_h2co_mm_spectrum.apex')
    sp.data *= 1/0.75 # T_A* -> T_MB
    sp.unit = "$T_{MB}$"
    # estimate the error from the data
    sp.error[:] = sp.stats((2.183e2,2.184e2))['std']

    # register the fitters
    sp.Registry.add_fitter('formaldehyde_mm_radex',
                           formaldehyde_radex_fitter,5)
    sp.Registry.add_fitter('formaldehyde_mm_radex_b',
                           formaldehyde_radex_fitter_b,5)
    sp.Registry.add_fitter('formaldehyde_mm_radex_both',
                           formaldehyde_radex_fitter_both,5)

    # make 3 copies so that we can view independent fits
    # This step isn't really necessary, but it's a nice way to compare the fits
    # side-by-side
    sp1 = sp.copy()
    sp2 = sp.copy()
    sp3 = sp.copy()

    sp1.plotter(figure=1)
    sp1.specfit(fittype='formaldehyde_mm_radex',

```

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```

        multifit=None,
        guesses=[100,13.2,4.5,0,7.0],
        limits=[(20,200),(11,15),(3,5.5),(-5,5),(2,15)],
        limited=[(True,True)]*5,
        fixed=[False,False,True,False,False],
        quiet=False,)
sp1.plotter.savefig('h2co_mm_fit_303-202_321-220.png')

sp2.plotter(figure=2)
sp2.specfit(fittype='formaldehyde_mm_radex_b',
            multifit=None,
            guesses=[100,13.2,4.5,0,7.0],
            limits=[(20,200),(11,15),(3,5.5),(-5,5),(2,15)],
            limited=[(True,True)]*5,
            fixed=[False,False,True,False,False],
            quiet=False,)
sp2.plotter.savefig('h2co_mm_fit_303-202_322-221.png')

# Do two versions of the fit with different input guesses
sp3.plotter(figure=3)
sp3.specfit(fittype='formaldehyde_mm_radex_both',
            multifit=None,
            guesses=[95,13.2,4.5,0,7.0],
            limits=[(20,200),(11,15),(3,5.5),(-5,5),(2,15)],
            limited=[(True,True)]*5,
            fixed=[True,False,False,False,False],
            quiet=False,)
sp3.plotter.savefig('h2co_mm_fit_303-202_322-221_and_303-202_321-220_try1.png')

sp3.plotter(figure=4)
sp3.specfit(fittype='formaldehyde_mm_radex_both',
            multifit=None,
            guesses=[105,13.2,4.5,0,7.0],
            limits=[(20,200),(11,15),(3,5.5),(-5,5),(2,15)],
            limited=[(True,True)]*5,
            fixed=[False,True,False,False,False],
            quiet=False,)
sp3.plotter.savefig('h2co_mm_fit_303-202_322-221_and_303-202_321-220_try2.png')

# An illustration of the degeneracy between parameters
sp3.plotter(figure=5)
sp3.specfit.plot_model([95,13.5,4.75,2.89,6.85])
sp3.specfit.plot_model([165,13.5,7.0,2.89,6.85],composite_fit_color='b')
sp3.specfit.plot_model([117,13.15,5.25,2.89,6.85],composite_fit_color='g')
sp3.plotter.savefig("h2co_mm_fit_degeneracy_example.png")

```

## 8.7 Radio Fitting: NH<sub>3</sub> example

```

import pyspeckit

# The ammonia fitting wrapper requires a dictionary specifying the transition name
# (one of the four specified below) and the filename. Alternately, you can have the
# dictionary values be pre-loaded Spectrum instances
filenames = {'oneone': 'G032.751-00.071_nh3_11_Tastar.fits',

```

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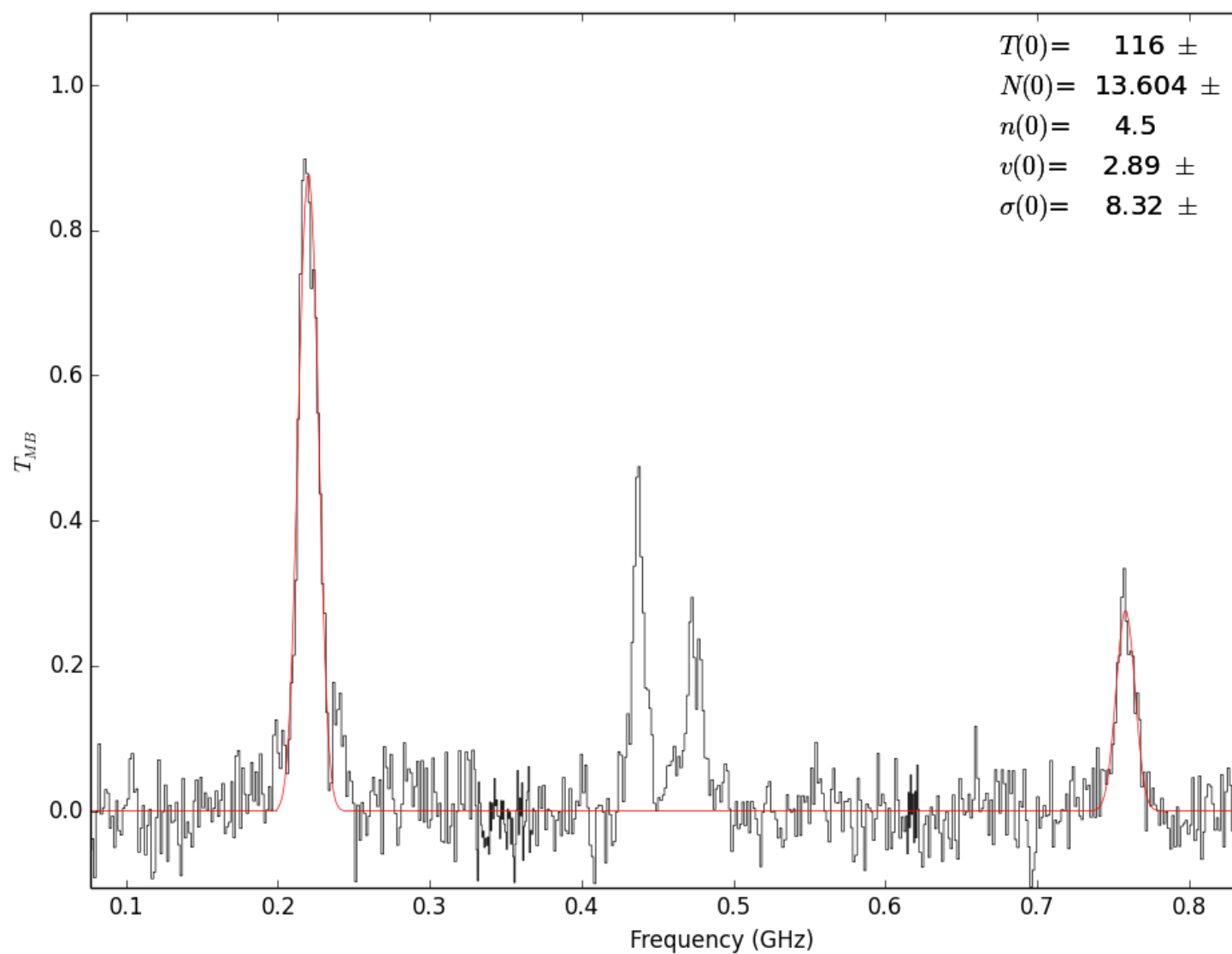


Fig. 2: Fit with the 302-202 and 321-220 lines

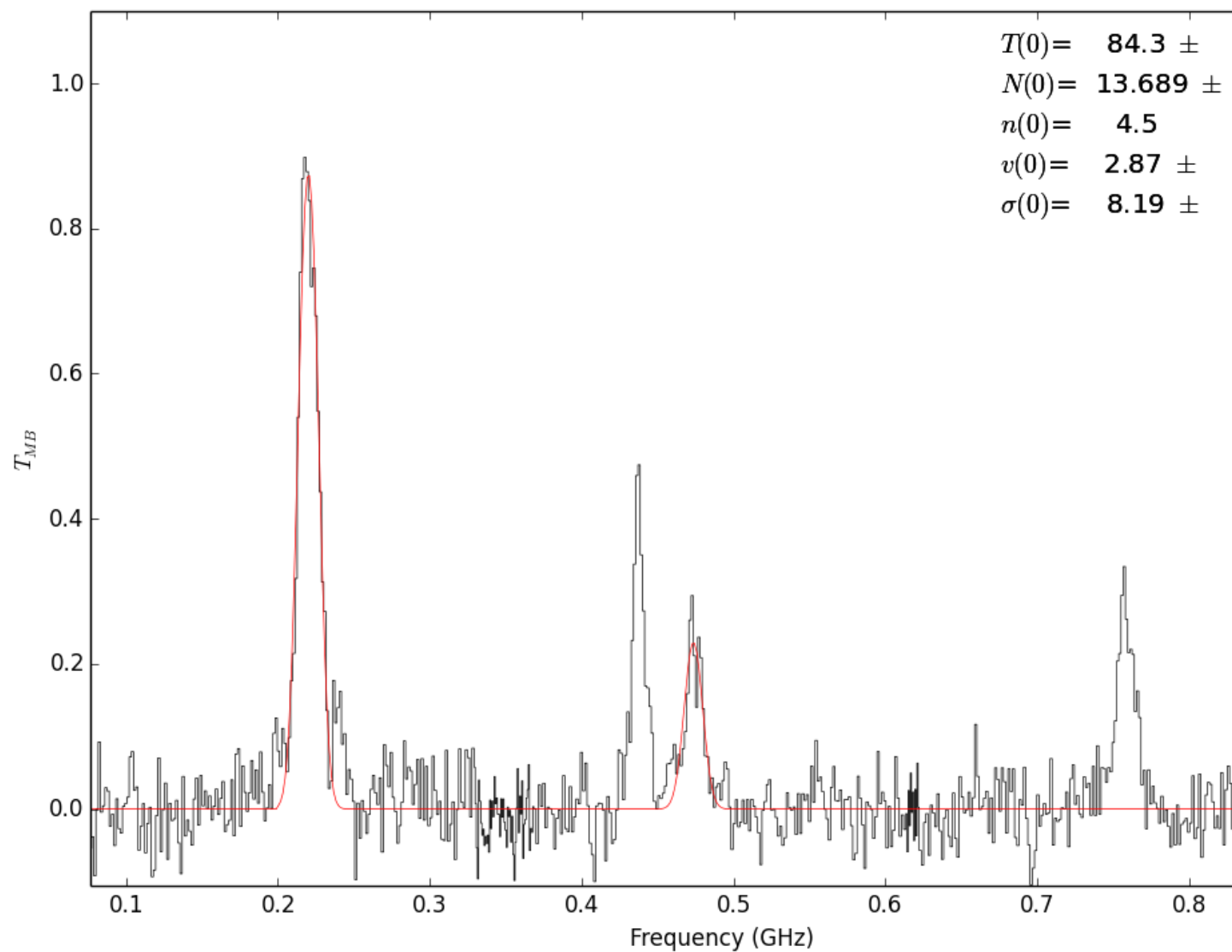


Fig. 3: Fit with the 302-202 and 321-220 lines



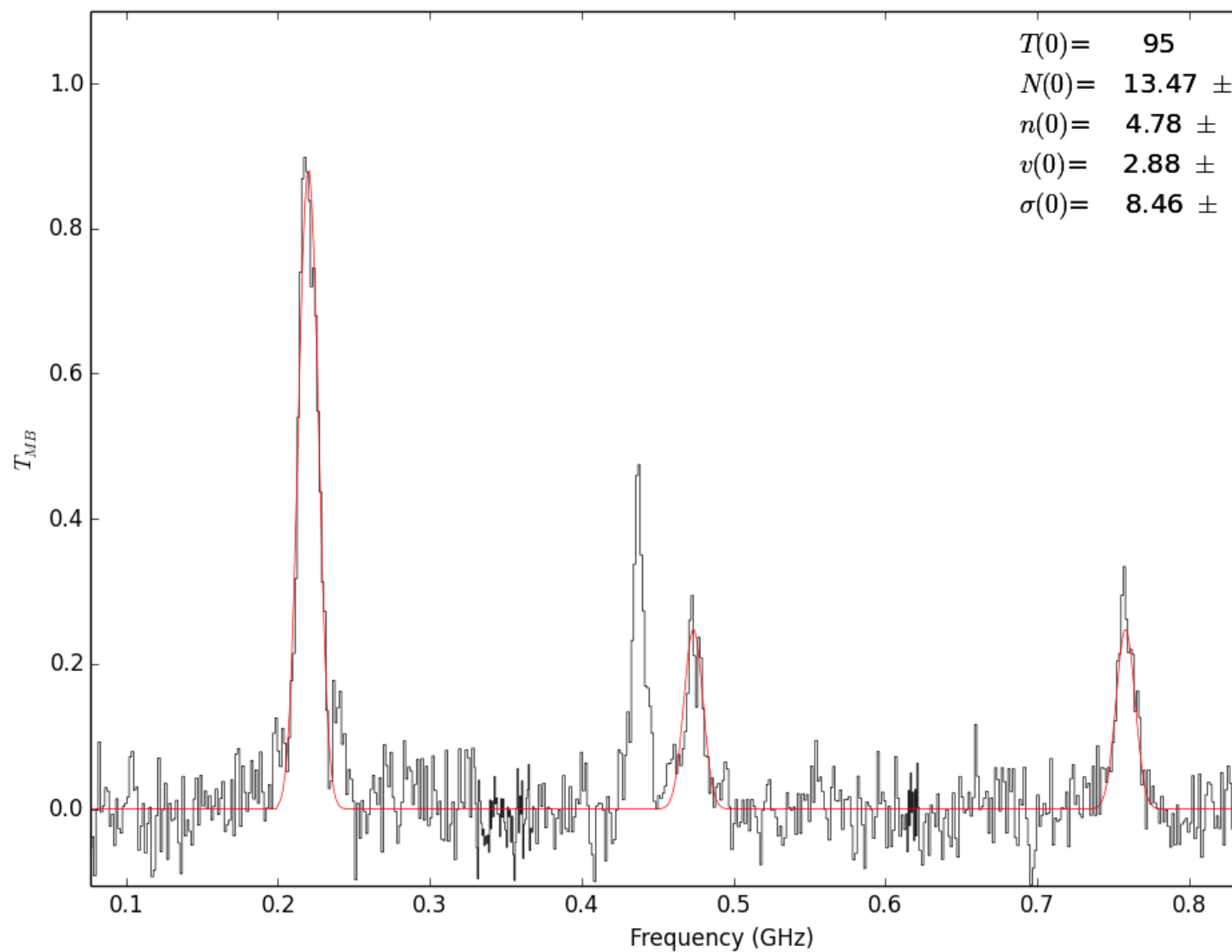


Fig. 4: Fit with all 3 lines. In this case, the temperature is unconstrained.

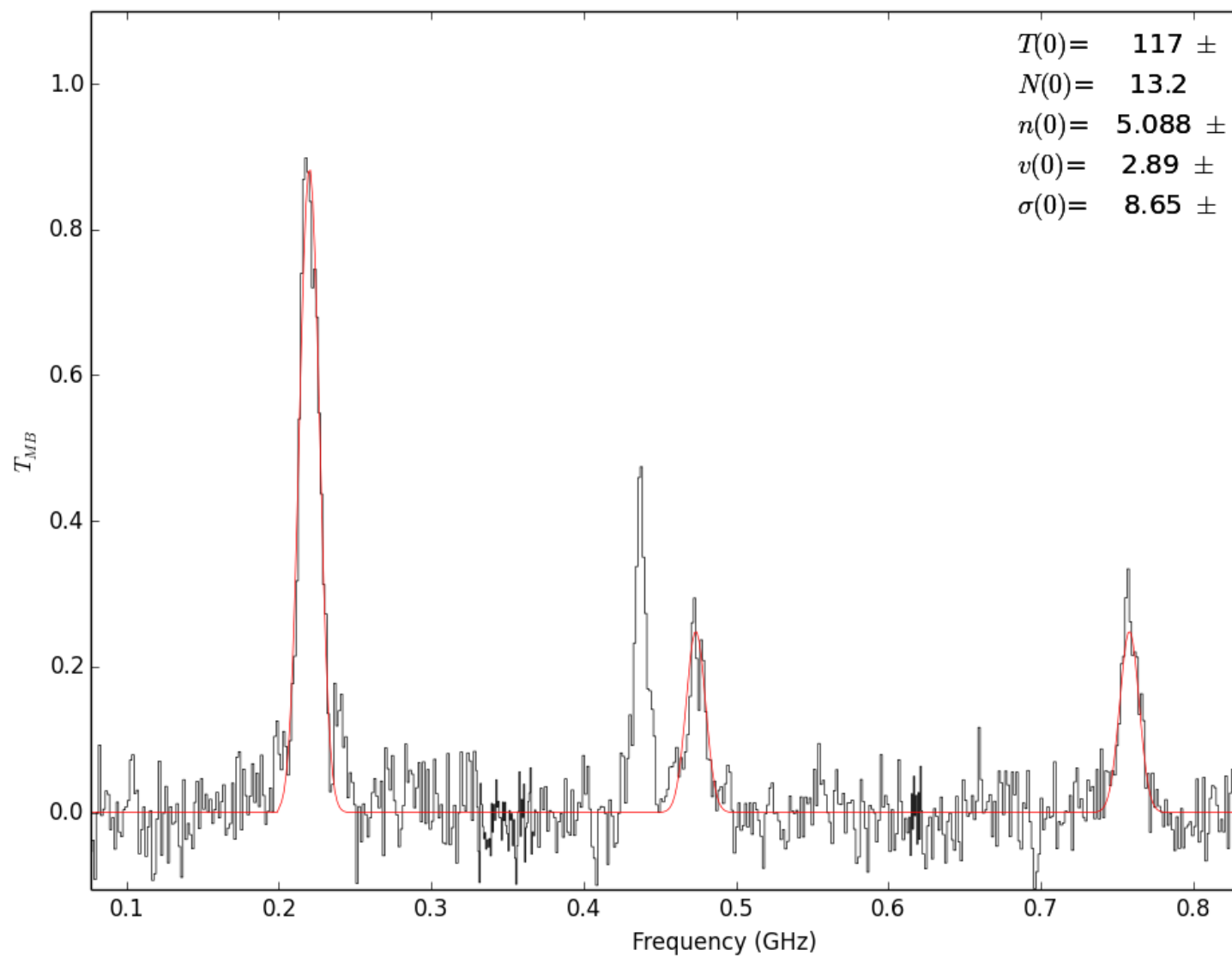


Fig. 5: Fit with all 3 lines. In this case, the column is unconstrained.

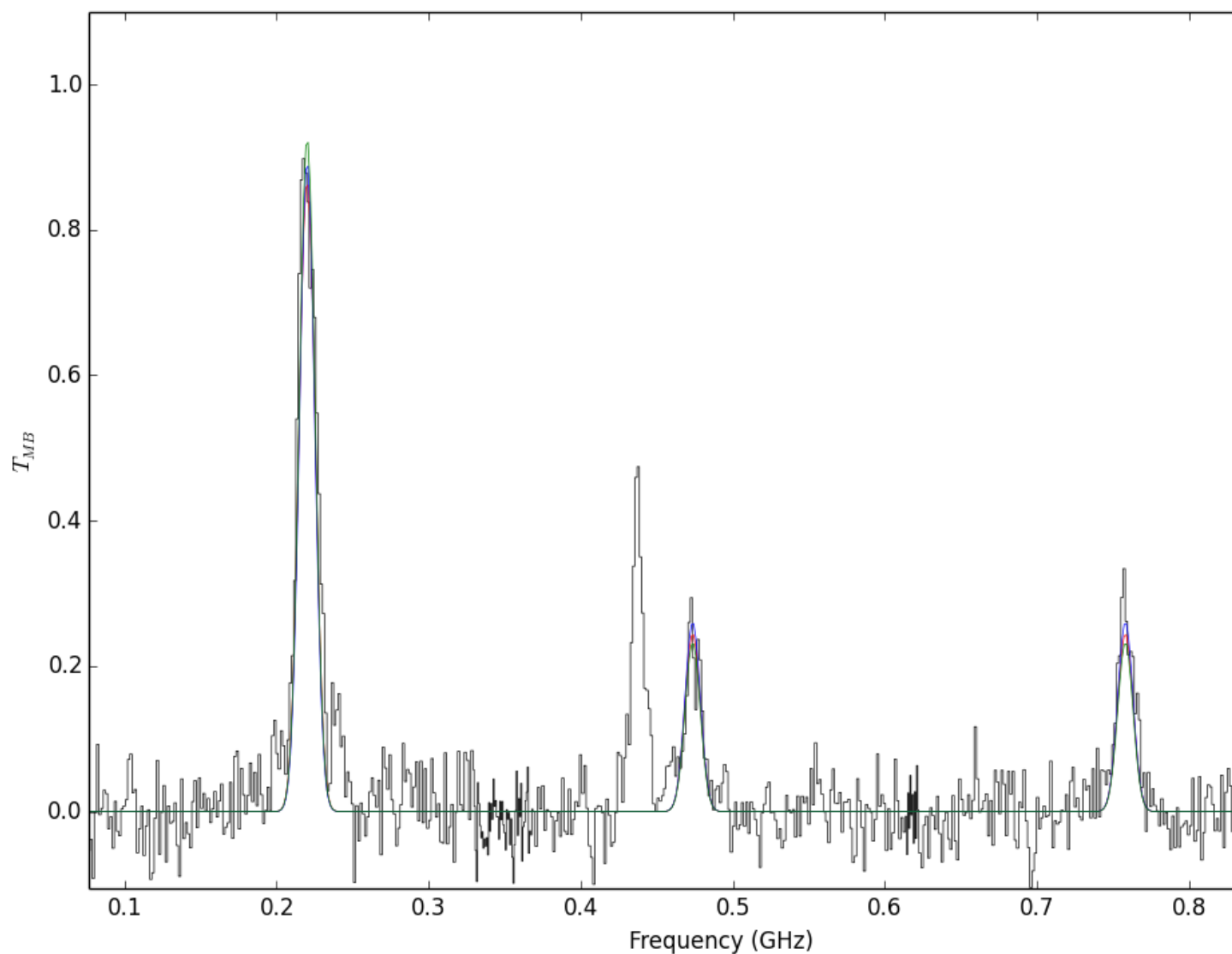


Fig. 6: A demonstration of degenerate parameters. The parameters used are:

- Blue:  $T, N, n = 95, 13.5, 4.75$
- Green:  $T, N, n = 165, 13.5, 7.0$
- Red:  $T, N, n = 117, 13.15, 5.25$

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```

'twotwo': 'G032.751-00.071_nh3_22_Tastar.fits',
'threethree': 'G032.751-00.071_nh3_33_Tastar.fits',
'fourfour': 'G032.751-00.071_nh3_44_Tastar.fits'}

# Fit the ammonia spectrum with some reasonable initial guesses. It is
# important to crop out extraneous junk and to smooth the data to make the
# fit proceed at a reasonable pace.
spdict1,spectra1 = pyspeckit.wrappers.fitnh3.fitnh3tkin(filenamees,crop=[0,80],tkin=18.65,tex=4.49,
↳column=15.5,fortho=0.9,verbose=False,smooth=6)

```

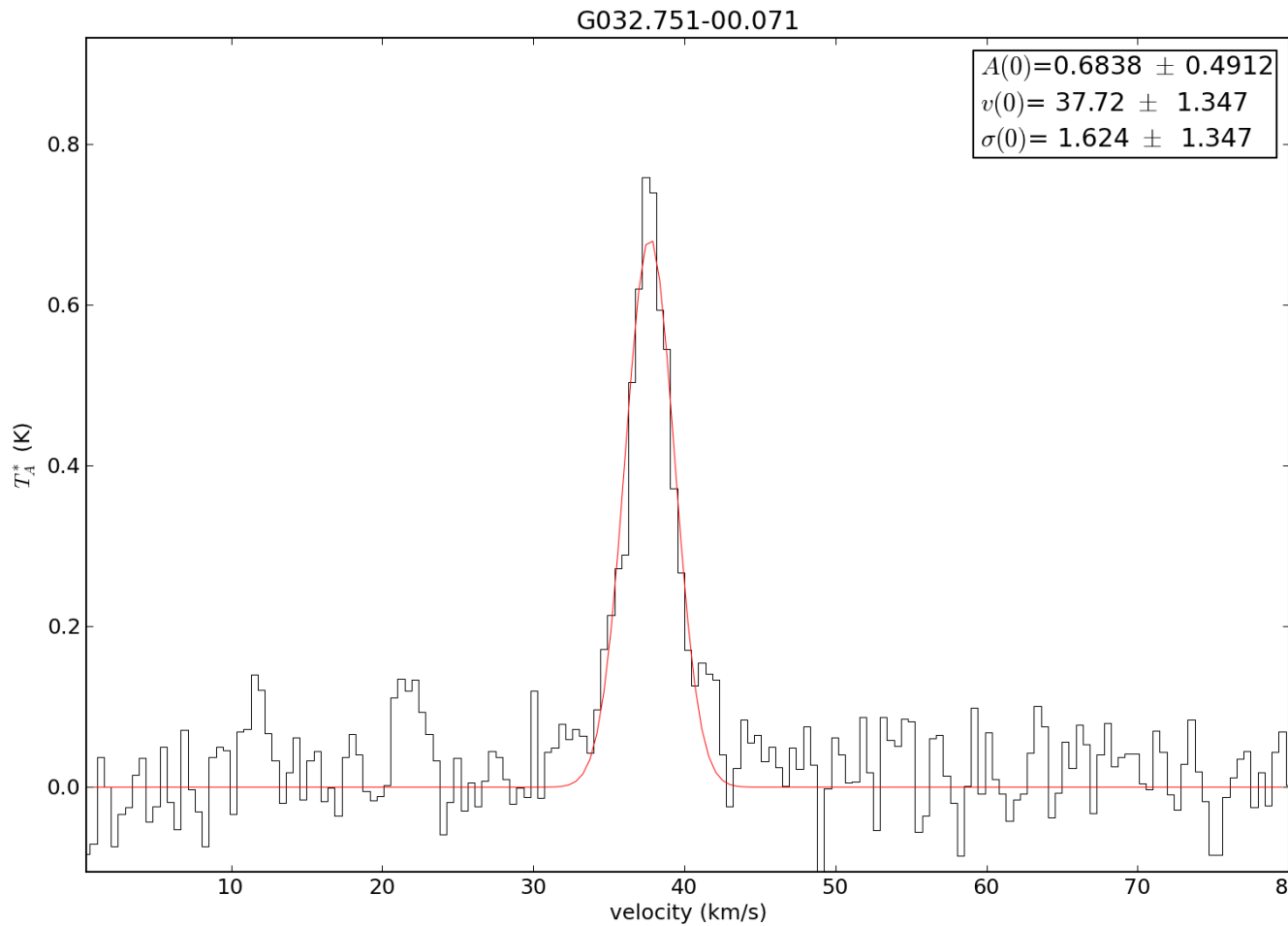


Fig. 7: The 2-2 transition is used to guess the central velocity and width via gaussian fitting because its hyperfine lines are weaker

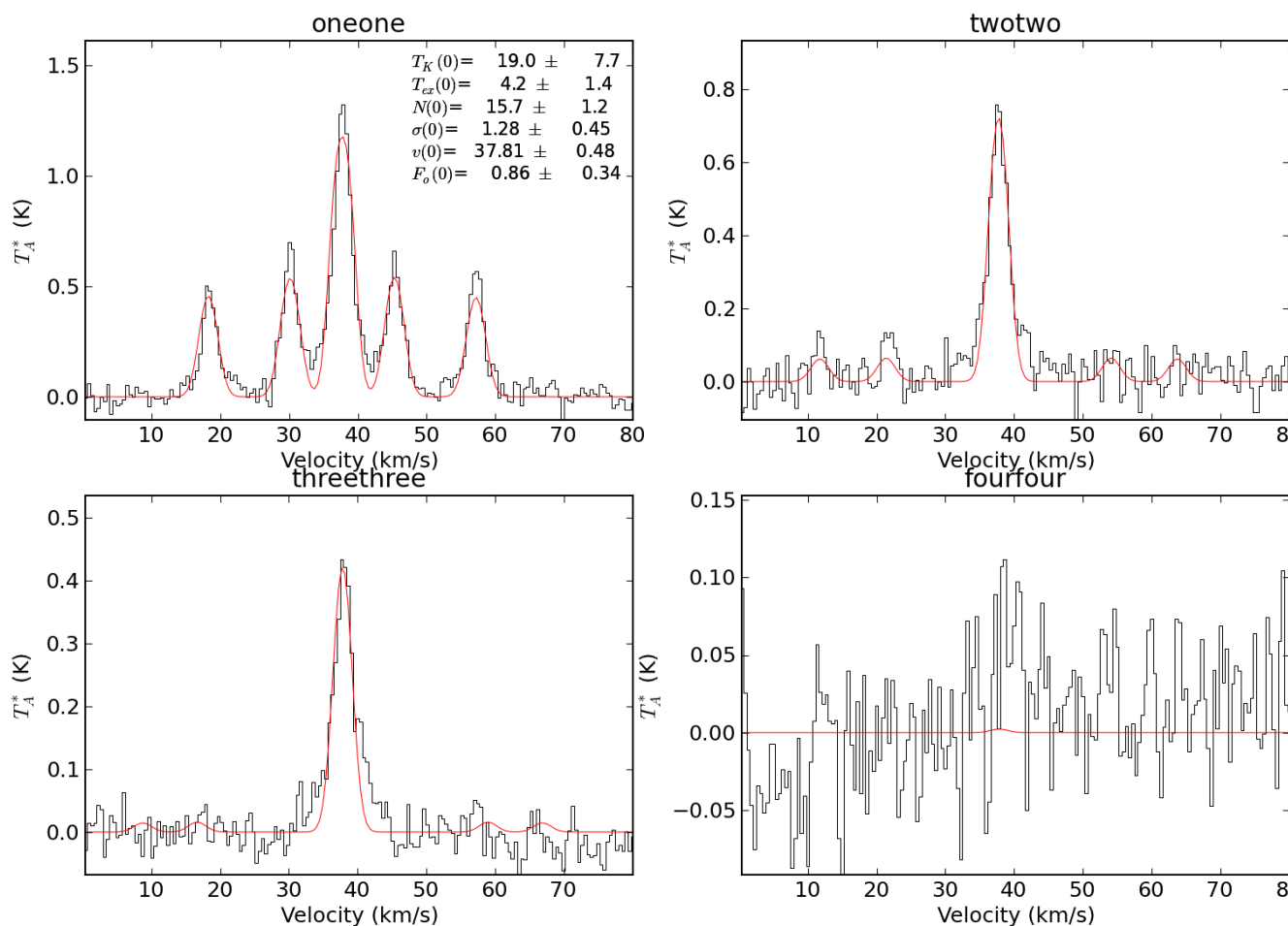


Fig. 8: Then all 4 lines are simultaneously fit. Even upper limits on the 4-4 line can provide helpful constraints on the model

## 8.8 Radio Fitting: NH<sub>3</sub> CUBE example

```

"""
Fit NH3 Cube
=====

Example script to fit all pixels in an NH3 data cube.

This is a bit of a mess, and fairly complicated (intrinsically),
but if you have matched 1-1 + 2-2 + ... NH3 cubes, you should be
able to modify this example and get something useful out.

.. WARNING:: Cube fitting, particularly with a complicated line profile
ammonia, can take a long time. Test this on a small cube first!

.. TODO:: Turn this example script into a function. But customizing
the fit parameters will still require digging into the data manually
(e.g., excluding bad velocities, or excluding the hyperfine lines from
the initial guess)
"""

import pyspeckit
import astropy
try:
    import astropy.io.fits as pyfits
except ImportError:
    import pyfits
import numpy as np
import os
from astropy.convolution import convolve_fft, Gaussian2DKernel

# set up CASA-like shortcuts
F=False; T=True

# Some optional parameters for the script
# (if False, it will try to load an already-stored version
# of the file)
fitcube = True

# Mask out low S/N pixels (to speed things up)
mask = pyfits.getdata('hotclump_11_mask.fits')
mask = np.isfinite(mask) * (mask > 0)

# Load the data using a mask
# Then calibrate the data (the data we're loading in this case are in Janskys,
# but we want surface brightness in Kelvin for the fitting process)
cube11 = pyspeckit.Cube('hotclump_11.cube_r0.5_rerun.image.fits', maskmap=mask)
cube11.cube *= (13.6 * (300.0 /
    (pyspeckit.spectrum.models.ammonia.freq_dict['oneone']/1e9))**2 *
    1./cube11.header.get('BMAJ')/3600. * 1./cube11.header.get('BMIN')/3600. )
cube11.unit = "K"
cube22 = pyspeckit.Cube('hotclump_22.cube_r0.5_contsub.image.fits', maskmap=mask)
cube22.cube *= (13.6 * (300.0 /
    (pyspeckit.spectrum.models.ammonia.freq_dict['twotwo']/1e9))**2 *
    1./cube22.header.get('BMAJ')/3600. * 1./cube22.header.get('BMIN')/3600. )
cube22.unit = "K"
cube44 = pyspeckit.Cube('hotclump_44.cube_r0.5_contsub.image.fits', maskmap=mask)
cube44.cube *= (13.6 * (300.0 /

```

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```

        (pyspeckit.spectrum.models.ammonia.freq_dict['fourfour']/1e9))**2 *
        1./cube44.header.get('BMAJ')/3600. * 1./cube44.header.get('BMIN')/3600. )
cube44.unit = "K"

# Compute an error map. We use the 1-1 errors for all 3 because they're
# essentially the same, but you could use a different error map for each
# frequency
oneonemomentfn = 'hotclump_11.cube_r0.5_rerun.image.moment_linefree.fits'
errmap11 = (pyfits.getdata(oneonemomentfn).squeeze() * 13.6 *
            (300.0 /
             (pyspeckit.spectrum.models.ammonia.freq_dict['oneone']/1e9))**2
            * 1./cube11.header.get('BMAJ')/3600. *
            1./cube11.header.get('BMIN')/3600.)
# Interpolate errors across NaN pixels
errmap11[errmap11 != errmap11] = convolve_fft(errmap11,
                                              Gaussian2DKernel(3),
                                              interpolate_nan=True)[errmap11 != errmap11]

# Stack the cubes into one big cube. The X-axis is no longer linear: there
# will be jumps from 1-1 to 2-2 to 4-4.
cubes = pyspeckit.CubeStack([cube11, cube22, cube44], maskmap=mask)
cubes.unit = "K"

# Make a "moment map" to contain the initial guesses
# If you've already fit the cube, just re-load the saved version
# otherwise, re-fit it
if os.path.exists('hot_momentcube.fits'):
    momentcubefile = pyfits.open('hot_momentcube.fits')
    momentcube = momentcubefile[0].data
else:
    cube11.mapplot()
    # compute the moment at each pixel
    cube11.momenteach()
    momentcube = cube11.momentcube
    momentcubefile = pyfits.PrimaryHDU(data=momentcube, header=cube11.header)
if astropy.version.major >= 2 or (astropy.version.major==1 and astropy.version.minor>=3):
    momentcubefile.writeto('hot_momentcube.fits', overwrite=True)
else:
    momentcubefile.writeto('hot_momentcube.fits', clobber=True)

# Create a "guess cube". Because we're fitting physical parameters in this
# case, we want to make the initial guesses somewhat reasonable
# As above, we'll just reload the saved version if it exists
guessfn = 'hot_guesscube.fits'
if os.path.exists(guessfn):
    guesscube = pyfits.open(guessfn)
    guesses = guesscube[0].data
else:
    guesses = np.zeros((6,) + cubes.cube.shape[1:])
    guesses[0, :, :] = 20 # Kinetic temperature
    guesses[1, :, :] = 5 # Excitation Temp
    guesses[2, :, :] = 14.5 # log(column)
    guesses[3, :, :] = momentcube[3, :, :] / 5 # Line width / 5 (the NH3 moment overestimates linewidth)
    guesses[4, :, :] = momentcube[2, :, :] # Line centroid
    guesses[5, :, :] = 0.5 # F(ortho) - ortho NH3 fraction (fixed)

```

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```

guesscube = pyfits.PrimaryHDU(data=guesses, header=cube11.header)
if astropy.version.major >= 2 or (astropy.version.major==1 and astropy.version.minor>=3):
    guesscube.writeto(guessfn, overwrite=True)
else:
    guesscube.writeto(guessfn, clobber=True)

# This bit doesn't need to be in an if statment
if fitcube:
    # excise guesses that fall out of the "good" range
    guesses[4,:,:][guesses[4,:,:] > 100] = 100.0
    guesses[4,:,:][guesses[4,:,:] < 91] = 95

    # do the fits
    # signal_cut means ignore any pixel with peak S/N less than this number
    # In this fit, many of the parameters are limited
    # start_from_point selects the pixel coordinates to start from
    # use_nearest_as_guess says that, at each pixel, the input guesses will be
    # set by the fitted parameters from the nearest pixel with a good fit
    # HOWEVER, because this fitting is done in parallel (multicore=12 means
    # 12 parallel fitting processes will run), this actually means that EACH
    # core will have its own sub-set of the cube that it will search for good
    # fits. So if you REALLY want consistency, you need to do the fit in serial.
    cubes.fiteach(fittype='ammonia', multifit=None, guesses=guesses,
        integral=False, verbose_level=3, fixed=[F,F,F,F,T], signal_cut=3,
        limitedmax=[F,F,F,F,T,T],
        maxpars=[0,0,0,0,101,1],
        limitedmin=[T,T,F,F,T,T],
        minpars=[2.73,2.73,0,0,91,0],
        use_nearest_as_guess=True, start_from_point=(94,250),
        multicore=12,
        errmap=errmap11)

    # Save the fitted parameters in a data cube
    fitcubefile = pyfits.PrimaryHDU(data=np.concatenate([cubes.parcube,cubes.errcube]), header=cubes.
header)
    fitcubefile.header.update('PLANE1','TKIN')
    fitcubefile.header.update('PLANE2','TEX')
    fitcubefile.header.update('PLANE3','COLUMN')
    fitcubefile.header.update('PLANE4','SIGMA')
    fitcubefile.header.update('PLANE5','VELOCITY')
    fitcubefile.header.update('PLANE6','FORTH0')
    fitcubefile.header.update('PLANE7','eTKIN')
    fitcubefile.header.update('PLANE8','eTEX')
    fitcubefile.header.update('PLANE9','eCOLUMN')
    fitcubefile.header.update('PLANE10','eSIGMA')
    fitcubefile.header.update('PLANE11','eVELOCITY')
    fitcubefile.header.update('PLANE12','eFORTH0')
    fitcubefile.header.update('CDELTA3',1)
    fitcubefile.header.update('CTYPE3','FITPAR')
    fitcubefile.header.update('CRVAL3',0)
    fitcubefile.header.update('CRPIX3',1)
    fitcubefile.writeto("hot_fitcube_try6.fits")
else: # you can read in a fit you've already done!
    cubes.load_model_fit('hot_fitcube_try6.fits', 6, 'ammonia', _temp_fit_loc=(94,250))
    cubes.specfit.parinfo[5]['fixed'] = True

```

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```
# Now do some plotting things
import pylab as pl

# Set the map-to-plot to be the line centroid
cubes.mapplot.plane = cubes.parcube[4,:,:]
cubes.mapplot(estimator=None,vmin=91,vmax=101)

# Set the reference frequency to be the 1-1 line frequency
cubes.xarr.refX = pyspeckit.spectrum.models.ammonia.freq_dict['oneone']
cubes.xarr.refX_unit='Hz'

# If you wanted to view the spectra in velocity units, use this:
#cubes.xarr.convert_to_unit('km/s')
#cubes.plotter.xmin=55
#cubes.plotter.xmax=135

# Now replace the cube's plotter with a "special" plotter
# The "special" plotter puts the 1-1, 2-2, and 4-4 lines in their own separate
# windows

cubes.plot_special = pyspeckit.wrappers.fitnh3.plotter_override
cubes.plot_special_kwargs = {'fignum':3, 'vrange':[55,135]}
cubes.plot_spectrum(160,99)

# make interactive
pl.ion()
pl.show()

# At this point, you can click on any pixel in the image and see the spectrum
# with the best-fit ammonia profile overlaid.
```

## 8.9 Radio fitting: NH3 multiple lines with independent tau, Tex

Example hyperfine line fitting for the NH3 1-1 through 3-3 lines, including making up a synthetic spectrum

```
import numpy as np
import pyspeckit
from astropy import units as u
from pyspeckit.spectrum.models import ammonia_constants, ammonia, ammonia_hf
from pyspeckit.spectrum.models.ammonia_constants import freq_dict
from pyspeckit.spectrum.units import SpectroscopicAxis, SpectroscopicAxes

# Step 1. Generate a synthetic spectrum.  Already have a real spectrum?  Skip
# to step 2!
# Generate a synthetic spectrum based off of 3 NH3 lines
# Note that they are converted to GHz first
xarr11 = SpectroscopicAxis(np.linspace(-30, 30, 100)*u.km/u.s,
                           velocity_convention='radio',
                           refX=freq_dict['oneone']).as_unit(u.GHz)
xarr22 = SpectroscopicAxis(np.linspace(-40, 40, 100)*u.km/u.s,
                           velocity_convention='radio',
                           refX=freq_dict['twotwo']).as_unit(u.GHz)
xarr33 = SpectroscopicAxis(np.linspace(-50, 50, 100)*u.km/u.s,
                           velocity_convention='radio',
```

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```

        refX=freq_dict['threethree']).as_unit(u.GHz)
# Merge the three X-axes into a single axis
xarr = SpectroscopicAxes([xarr11,xarr22,xarr33])

# Compute a synthetic model that is made of two temperature components with
# identical velocities
synthspec = (ammonia.ammonia(xarr, trot=20, ntot=15, fortho=0.5, xoff_v=0.0,
                             width=1.0) +
             ammonia.ammonia(xarr, trot=50, ntot=14, fortho=0.5, xoff_v=0.0,
                             width=1.0))

# Create the Spectrum object
spectrum = pyspeckit.Spectrum(xarr=xarr, data=synthspec, header={})

# Step 2. You have a spectrum.
# plot it
spectrum.plotter()

# Use the multi-tex/multi-tau model generator to build up a model function
# You can use any set of oneone, twotwo, ..., eighteight (no 9-9 or higher)
# This sets the number of parameters to be fit: 2+2*(n_transitions)
fitter = ammonia_hf.nh3_vtau_multimodel_generator(['oneone', 'twotwo',
                                                  'threethree'])

# Register the fitter - i.e., tell pyspeckit where it is and how to use it
spectrum.specfit.Registry.add_fitter('nh3_vtau_123', fitter, fitter.npars)
# These are the parameter names, approximately:
# parnames=['center','width','Tex11','tau11','Tex22','tau22','Tex33','tau33'],

# Need to give some input guesses. We start with something wrong-ish: -5 km/s,
# 1.2 km/s width, and 15 K + 0.5 tau for all 3 lines
guesses = [-5, 1.2, 15, 0.5, 15, 0.5, 15, 0.5,]

# Plot up the guessed model
spectrum.plotter.axis.plot(spectrum.xarr,
                           fitter.n_modelfunc(guesses)(spectrum.xarr), 'b')

# Run the fit!
spectrum.specfit(fittype='nh3_vtau_123', guesses=guesses)

# display the correct and fitted answers
print("Low column version:")
def printthings(ammonia=ammonia.ammonia, xarr=xarr):
    print("Real optical depths of component 1: ",[ammonia(xarr, trot=20,
                                                         ntot=15, fortho=0.5,
                                                         xoff_v=0.0,
                                                         width=1.0,
                                                         return_tau=True)[x]
                                                         for x in ['oneone', 'twotwo',
                                                         'threethree']])
    print("Real optical depths of component 2: ",[ammonia(xarr, trot=50,
                                                         ntot=14, fortho=0.5,
                                                         xoff_v=0.0,
                                                         width=1.0,
                                                         return_tau=True)[x]
                                                         for x in ['oneone', 'twotwo',

```

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```

                                'threethree']])
printthings()

print("Fitted parameters: ", spectrum.specfit.parinfo)

# It works, but the covariances between tex and tau are large.
# So, another example with higher tau (and therefore... less degenerate?)

synthspec = (ammonia.ammonia(xarr, trot=20, ntot=16, fortho=0.5, xoff_v=0.0,
                             width=1.0) +
             ammonia.ammonia(xarr, trot=50, ntot=15, fortho=0.5, xoff_v=0.0,
                             width=1.0))
spectrum2 = pyspeckit.Spectrum(xarr=xarr, data=synthspec, header={})
spectrum2.plotter()
spectrum2.specfit.Registry.add_fitter('nh3_vtau_123', fitter, fitter.npars)
spectrum2.specfit(fittype='nh3_vtau_123', guesses=guesses)

# We can also examine what tau really should have been... kinda.
print("High column version:")
def printthings(ammonia=ammonia.ammonia, xarr=xarr):
    print("Real optical depths of component 1: ", [ammonia(xarr, trot=20,
                                                         ntot=16, fortho=0.5,
                                                         xoff_v=0.0,
                                                         width=1.0,
                                                         return_tau=True)[x]
                                                         for x in ['oneone', 'twotwo',
                                                         'threethree']])
    print("Real optical depths of component 2: ", [ammonia(xarr, trot=50,
                                                         ntot=15, fortho=0.5,
                                                         xoff_v=0.0,
                                                         width=1.0,
                                                         return_tau=True)[x]
                                                         for x in ['oneone', 'twotwo',
                                                         'threethree']])

printthings()
print("Fitted parameters: ", spectrum2.specfit.parinfo)

```

## 8.10 Radio Fitting: N<sub>2</sub>H<sup>+</sup> example

Example hyperfine line fitting for the N<sub>2</sub>H<sup>+</sup> 1-0 line.

```

import pyspeckit

# Load the spectrum
sp = pyspeckit.Spectrum('n2hp_opha_example.fits')

# Register the fitter
# The N2H+ fitter is 'built-in' but is not registered by default; this example
# shows how to register a fitting procedure
# 'multi' indicates that it is possible to fit multiple components and a
# background will not automatically be fit 4 is the number of parameters in the
# model (excitation temperature, optical depth, line center, and line width)
sp.Registry.add_fitter('n2hp_vtau', pyspeckit.models.n2hp.n2hp_vtau_fitter, 4)
sp.xarr.velocity_convention = 'radio'

```

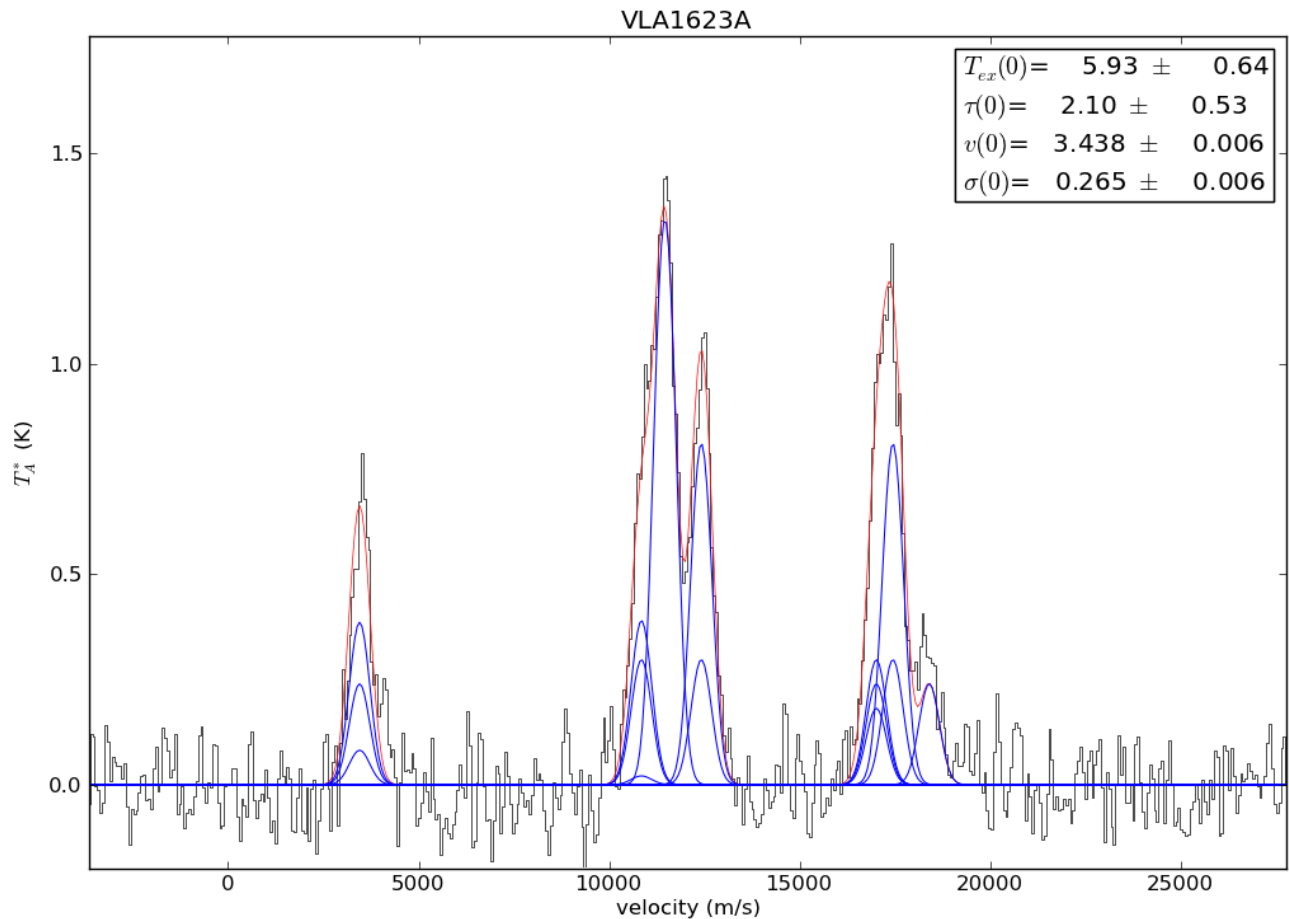
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```
# Run the fitter
sp.specfit(fittype='n2hp_vtau',multifit=None,guesses=[15,2,4,0.2])

# Plot the results
sp.plotter()
# Re-run the fitter (to get proper error bars) and show the individual fit components
sp.specfit(fittype='n2hp_vtau', multifit=None, guesses=[15, 2, 4, 0.2],
          show_hyperfine_components=True)

# Save the figure (this step is just so that an image can be included on the web page)
sp.plotter.savefig('n2hp_ophA_fit.png')
```



## 8.11 Radio Fitting: N<sub>2</sub>H<sup>+</sup> cube example

Example hyperfine line fitting of a data cube for the N<sub>2</sub>H<sup>+</sup> 1-0 line.

```
import astropy
import pyspeckit
import os
import astropy.units as u
import warnings
```

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```

from astropy import wcs

if not os.path.exists('n2hp_cube.fits'):
    import astropy.utils.data as aud
    from astropy.io import fits

    try:
        f = aud.download_file('ftp://cdsarc.u-strasbg.fr/pub/cats/J/A%2BA/472/519/fits/opha_n2h.fits')
    except Exception as ex:
        # this might be any number of different timeout errors (urllib2.URLError, socket.timeout, etc)
        # travis-ci can't handle ftp:
        # https://blog.travis-ci.com/2018-07-23-the-tale-of-ftp-at-travis-ci
        print("Failed to download from ftp. Exception was: {}".format(ex))
        f = aud.download_file('http://cdsarc.u-strasbg.fr/ftp/cats/J/A+A/472/519/fits/opha_n2h.fits')

    with fits.open(f) as ff:
        ff[0].header['CUNIT3'] = 'm/s'
        for kw in ['CTYPE4', 'CRVAL4', 'CDELTA4', 'CRPIX4', 'CROTA4']:
            if kw in ff[0].header:
                del ff[0].header[kw]
        ff.writeto('n2hp_cube.fits')

# Load the spectral cube cropped in the middle for efficiency
with warnings.catch_warnings():
    warnings.filterwarnings('ignore', category=wcs.FITSFIXEDWARNING)
    spc = pyspeckit.Cube('n2hp_cube.fits')[25:28, 12:15]
# Set the velocity convention: in the future, this may be read directly from
# the file, but for now it cannot be.
spc.xarr.refX = 93176265000.0*u.Hz
spc.xarr.velocity_convention = 'radio'
spc.xarr.convert_to_unit('km/s')

# Register the fitter
# The N2H+ fitter is 'built-in' but is not registered by default; this example
# shows how to register a fitting procedure
# 'multi' indicates that it is possible to fit multiple components and a
# background will not automatically be fit 4 is the number of parameters in the
# model (excitation temperature, optical depth, line center, and line width)
spc.Registry.add_fitter('n2hp_vtau', pyspeckit.models.n2hp.n2hp_vtau_fitter, 4)

# Get a measurement of the error per pixel
errmap = spc.slice(20, 28, unit='km/s').cube.std(axis=0)

# A good way to write a cube fitter is to have it load from disk if the cube
# fit was completed successfully in the past
if os.path.exists('n2hp_fitted_parameters.fits'):
    spc.load_model_fit('n2hp_fitted_parameters.fits', npars=4, npeaks=1)
else:
    # Run the fitter
    # Estimated time to completion ~ 2 minutes
    spc.fiteach(fittype='n2hp_vtau',
               guesses=[5, 0.5, 3, 1], # Tex=5K, tau=0.5, v_center=12, width=1 km/s
               signal_cut=3, # minimize the # of pixels fit for the example
               start_from_point=(2, 2), # start at a pixel with signal
               errmap=errmap,
               )
    # There are a huge number of parameters for the fiteach procedure. See:

```

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```

# http://pyspeckit.readthedocs.org/en/latest/example_nh3_cube.html
# http://pyspeckit.readthedocs.org/en/latest/cubes.html?highlight=fiteach#pyspeckit.cubes.
↪SpectralCube.Cube.fiteach
#
# Unfortunately, a complete tutorial on this stuff is on the to-do list;
# right now the use of many of these parameters is at a research level.
# However, pyspeckit@gmail.com will support them! They are being used
# in current and pending publications

# Save the fitted parameters to a FITS file, and overwrite one if one exists
spc.write_fit('n2hp_fitted_parameters.fits', overwrite=True)

# Show an integrated image
spc.mapplot()
# you can click on any pixel to see its spectrum & fit

# plot one of the fitted spectra
spc.plot_spectrum(2, 2, plot_fit=True)
# spc.parcube[:,27,14] = [ 14.82569198,  1.77055642,  3.15740051,  0.16035407]
# Note that the optical depth is the "total" optical depth, which is
# distributed among 15 hyperfine components. You can see this in
# pyspeckit.spectrum.models.n2hp.line_strength_dict
# As a sanity check, you can see that the brightest line has 0.259 of the total
# optical depth, so the peak line brightness is:
# (14.825-2.73) * (1-np.exp(-1.77 * 0.259)) = 4.45
# which matches the peak of 4.67 pretty well

# Show an image of the best-fit velocity
spc.mapplot.plane = spc.parcube[2,:,:]
spc.mapplot(estimator=None)

# running in script mode, the figures won't show by default on some systems
# import pylab as pl
# pl.draw()
# pl.show()

```

## 8.12 Radio Fitting: HCN example with freely varying hyperfine amplitudes

Example hyperfine line fitting for the HCN 1-0 line.

```

from __future__ import print_function
import pyspeckit
import pylab as pl
import astropy.units as u

# Load the spectrum & properly identify the units
# The data is from http://adsabs.harvard.edu/abs/1999A%26A...348..600P
sp = pyspeckit.Spectrum('02232_plus_6138.txt')
sp.xarr.set_unit(u.km/u.s)
sp.xarr.refX = 88.63184666e9 * u.Hz
sp.xarr.velocity_convention = 'radio'
sp.xarr.xtype='velocity'

```

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```

sp.unit='$T_A^*$'

# set the error array based on a signal-free part of the spectrum
sp.error[:] = sp.stats((-35,-25))['std']
# Register the fitter
# The HCN fitter is 'built-in' but is not registered by default; this example
# shows how to register a fitting procedure
# 'multi' indicates that it is possible to fit multiple components and a
# background will not automatically be fit
# 5 is the number of parameters in the model (line center,
# line width, and amplitude for the 0-1, 2-1, and 1-1 lines)
sp.Registry.add_fitter('hcn_varyhf', pyspeckit.models.hcn.hcn_varyhf_amp_fitter, 5)

# This one is the same, but with fixed relative amplitude hyperfine components
sp.Registry.add_fitter('hcn_fixedhf', pyspeckit.models.hcn.hcn_amp, 3)

# Plot the results
sp.plotter()
# Run the fixed-amplitude fitter and show the individual fit components
sp.specfit(fittype='hcn_fixedhf',
           multifit=None,
           guesses=[1,-48,0.6],
           show_hyperfine_components=True)
# Now plot the residuals offset below the original
sp.specfit.plotresiduals(axis=sp.plotter.axis, clear=False, yoffset=-1, color='g', label=False)
sp.plotter.reset_limits(ymin=-2)

# Save the figure (this step is just so that an image can be included on the web page)
sp.plotter.savefig('hcn_fixedhf_fit.png')

# Run the variable-amplitude fitter and show the individual fit components
# Note the different order of the arguments (velocity, width, then three amplitudes)
sp.specfit(fittype='hcn_varyhf',
           multifit=None,
           guesses=[-48,1,0.2,0.6,0.3],
           show_hyperfine_components=True,
           clear=True)

# Again plot the residuals
sp.specfit.plotresiduals(axis=sp.plotter.axis, clear=False, yoffset=-1, color='g', label=False)
sp.plotter.reset_limits(ymin=-2)

# Save the figure
sp.plotter.savefig('hcn_freehf_fit.png')

# now do the same thing, but allow the widths to vary too
# there are 7 parameters:
# 1. the centroid
# 2,3,4 - the amplitudes of the 0-1, 2-1, and 1-1 lines
# 5,6,7 - the widths of the 0-1, 2-1, and 1-1 lines
sp.Registry.add_fitter('hcn_varyhf_width', pyspeckit.models.hcn.hcn_varyhf_amp_width_fitter, 7)

# Run the fitter
sp.specfit(fittype='hcn_varyhf_width',
           multifit=None,

```

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```

        guesses=[-48,0.2,0.6,0.3,1,1,1],
        show_hyperfine_components=True,
        clear=True)

# print the fitted parameters:
print(sp.specfit.parinfo)
# Param #0      CENTER0 =      -51.865 +/-      0.0525058
# Param #1      AMP10-010 =      1.83238 +/-      0.0773993   Range:  [0,inf)
# Param #2      AMP12-010 =      5.26566 +/-      0.0835981   Range:  [0,inf)
# Param #3      AMP11-010 =      3.02621 +/-      0.0909095   Range:  [0,inf)
# Param #4      WIDTH10-010 =      2.16711 +/-      0.118651   Range:  [0,inf)
# Param #5      WIDTH12-010 =      1.90987 +/-      0.0476163   Range:  [0,inf)
# Param #6      WIDTH11-010 =      1.64409 +/-      0.076998   Range:  [0,inf)

sp.specfit.plotresiduals(axis=sp.plotter.axis,clear=False,yoffset=-1,color='g',label=False)
sp.plotter.reset_limits(ymin=-2)

# Save the figure (this step is just so that an image can be included on the web page)
sp.plotter.savefig('hcn_freehf_ampandwidth_fit.png')

# Finally, how well does a 2-component fit work?
sp.specfit(fittype='hcn_fixedhf',
           multifit=None,
           guesses=[1,-48,0.6,0.1,-46,0.6],
           show_hyperfine_components=True,
           clear=True)
sp.specfit.plotresiduals(axis=sp.plotter.axis,clear=False,yoffset=-1,color='g',label=False)
sp.plotter.reset_limits(ymin=-2)

# Save the figure (this step is just so that an image can be included on the web page)
sp.plotter.savefig('hcn_fixedhf_fit_2components.png')

```

The green lines in the following figures all show the residuals to the fit

## 8.13 Simple Radio Fitting: HCO+ example

```

import pyspeckit

# load a FITS-compliant spectrum
spec = pyspeckit.Spectrum('10074-190_HCOp.fits')
# The units are originally frequency (check this by printing spec.xarr.units).
# I want to know the velocity. Convert!
# Note that this only works because the reference frequency is set in the header
spec.xarr.convert_to_unit('km/s')

# plot it
spec.plotter()

# Subtract a baseline
spec.baseline()

# Fit a gaussian. We know it will be an emission line, so we force a positive guess
spec.specfit(negamp=False)

```

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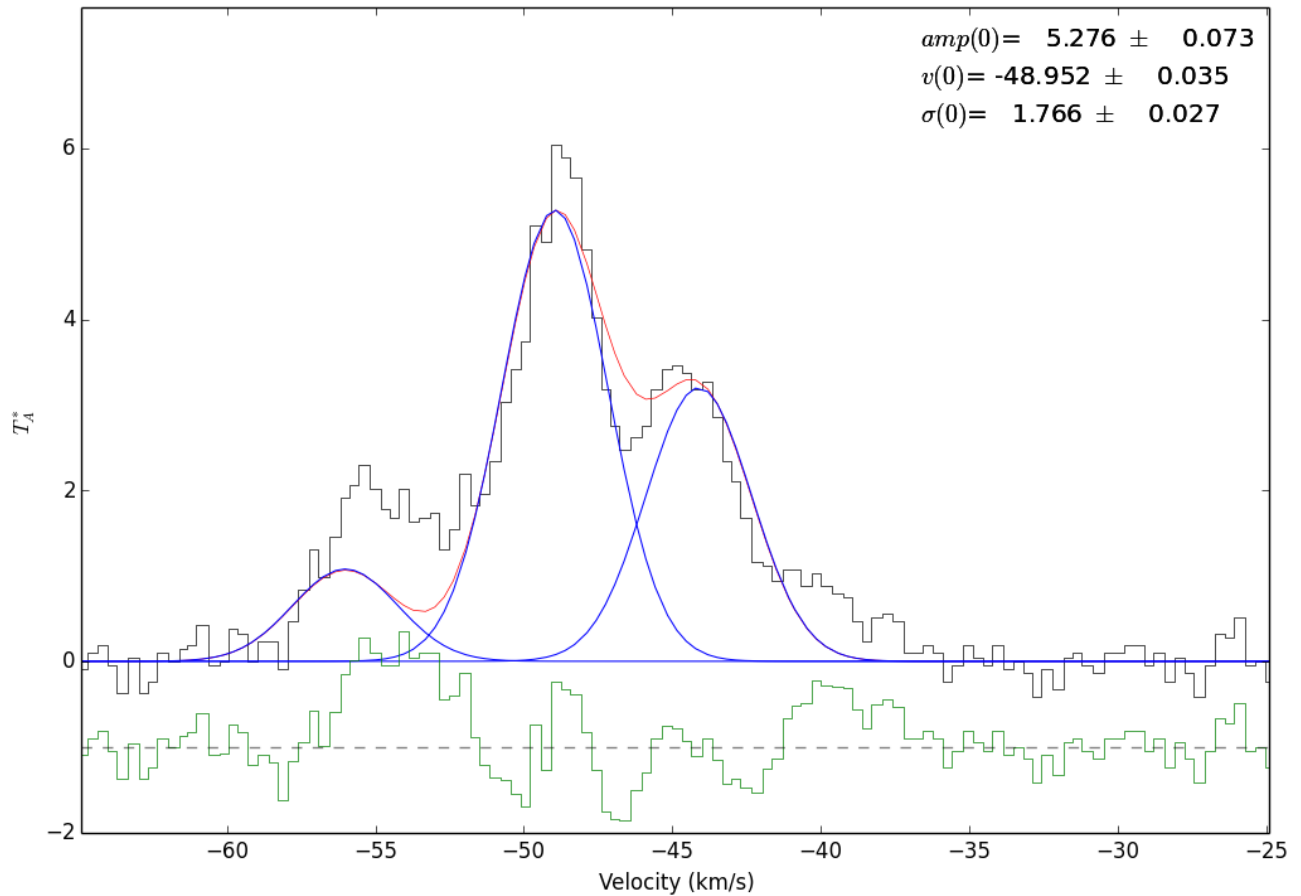


Fig. 9: Fit to the 3 hyperfine components of HCN 1-0 simultaneously with fixed amplitudes. The (0)'s indicate that this is the 0<sup>th</sup> velocity component being fit (though that velocity corresponds to the 12-01 component of the line)

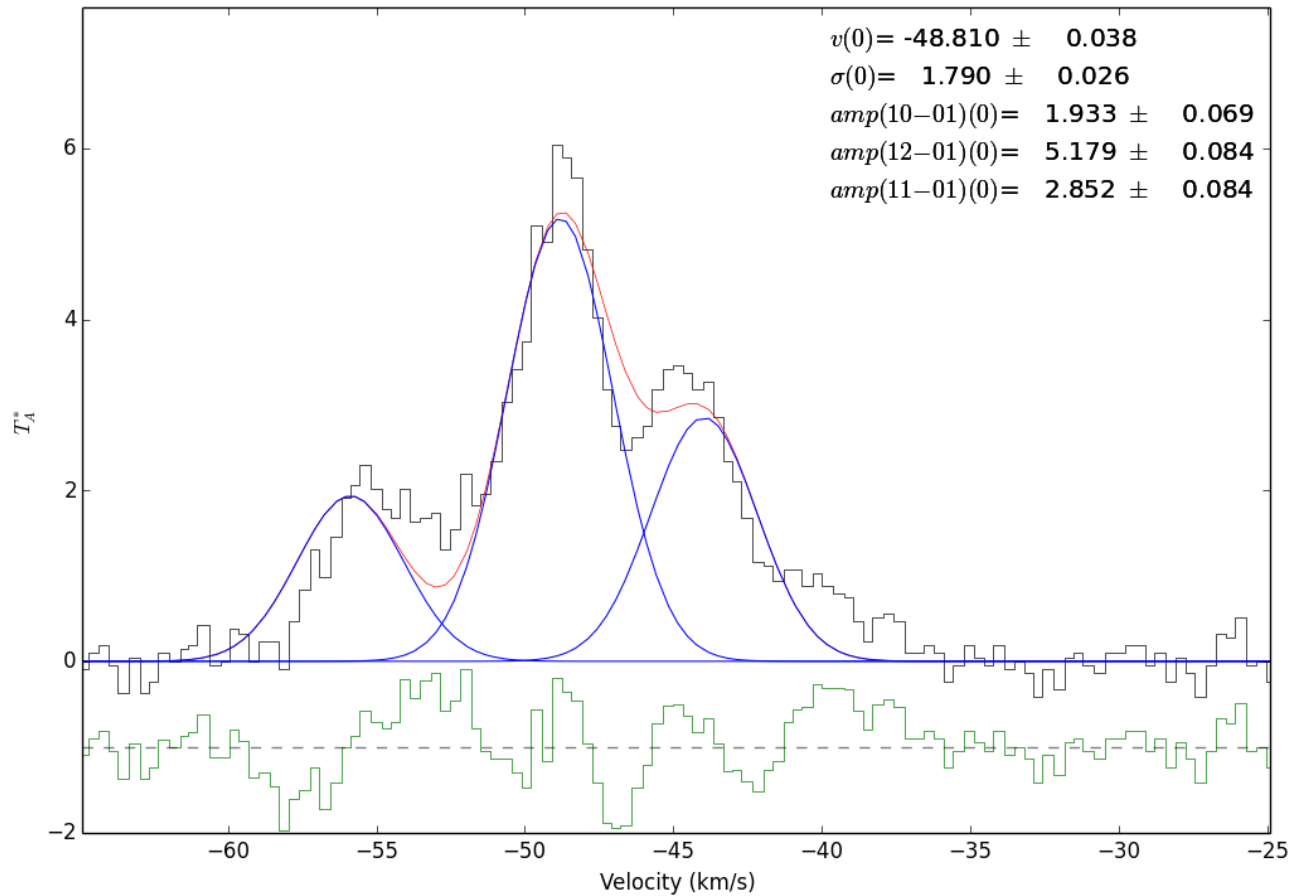


Fig. 10: Fit to the 3 hyperfine components of HCN 1-0 simultaneously with freely varying amplitudes. The (0)'s indicate that this is the 0'th velocity component being fit

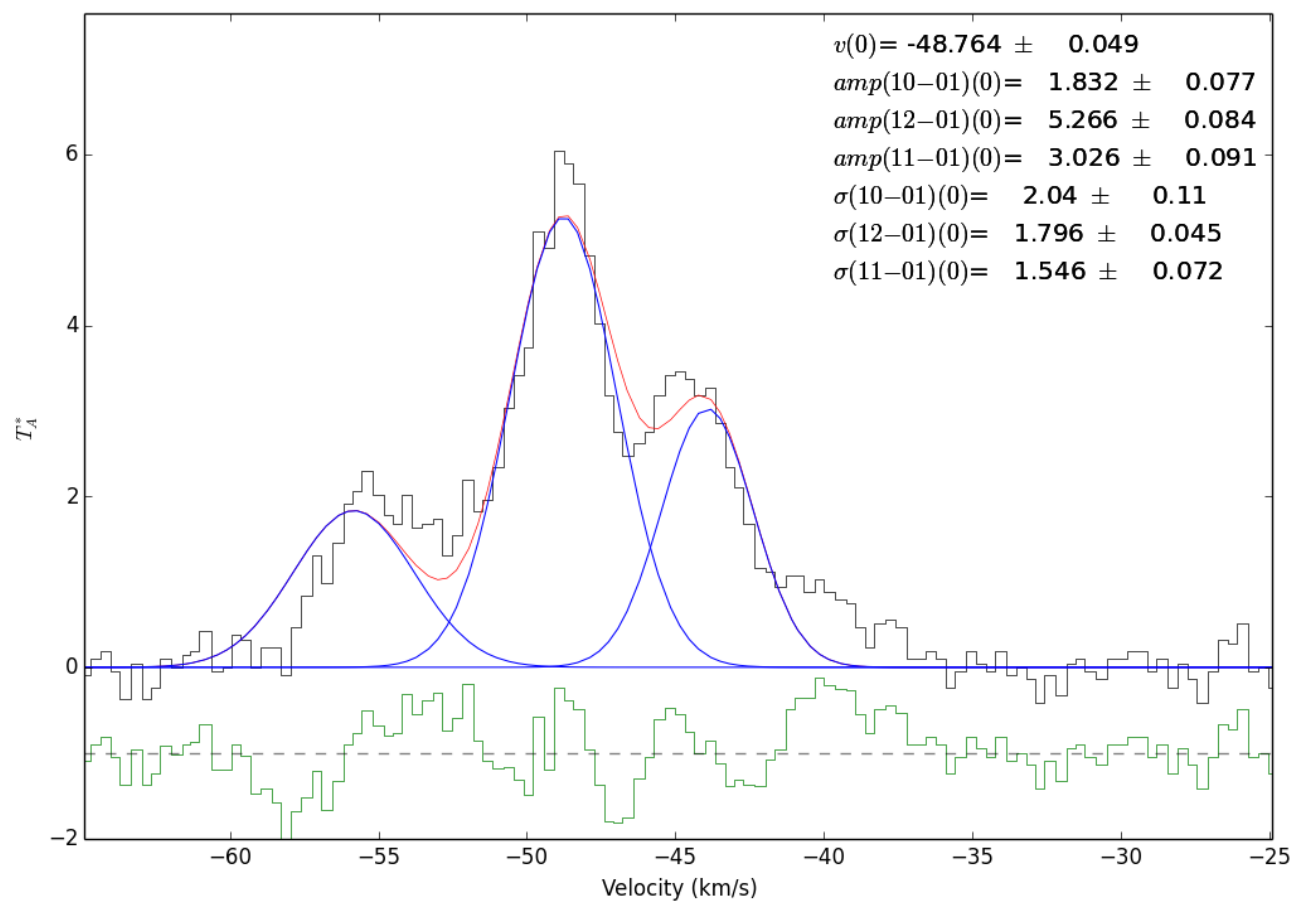


Fig. 11: Fit to the 3 hyperfine components of HCN 1-0 simultaneously. The widths are allowed to vary in this example.

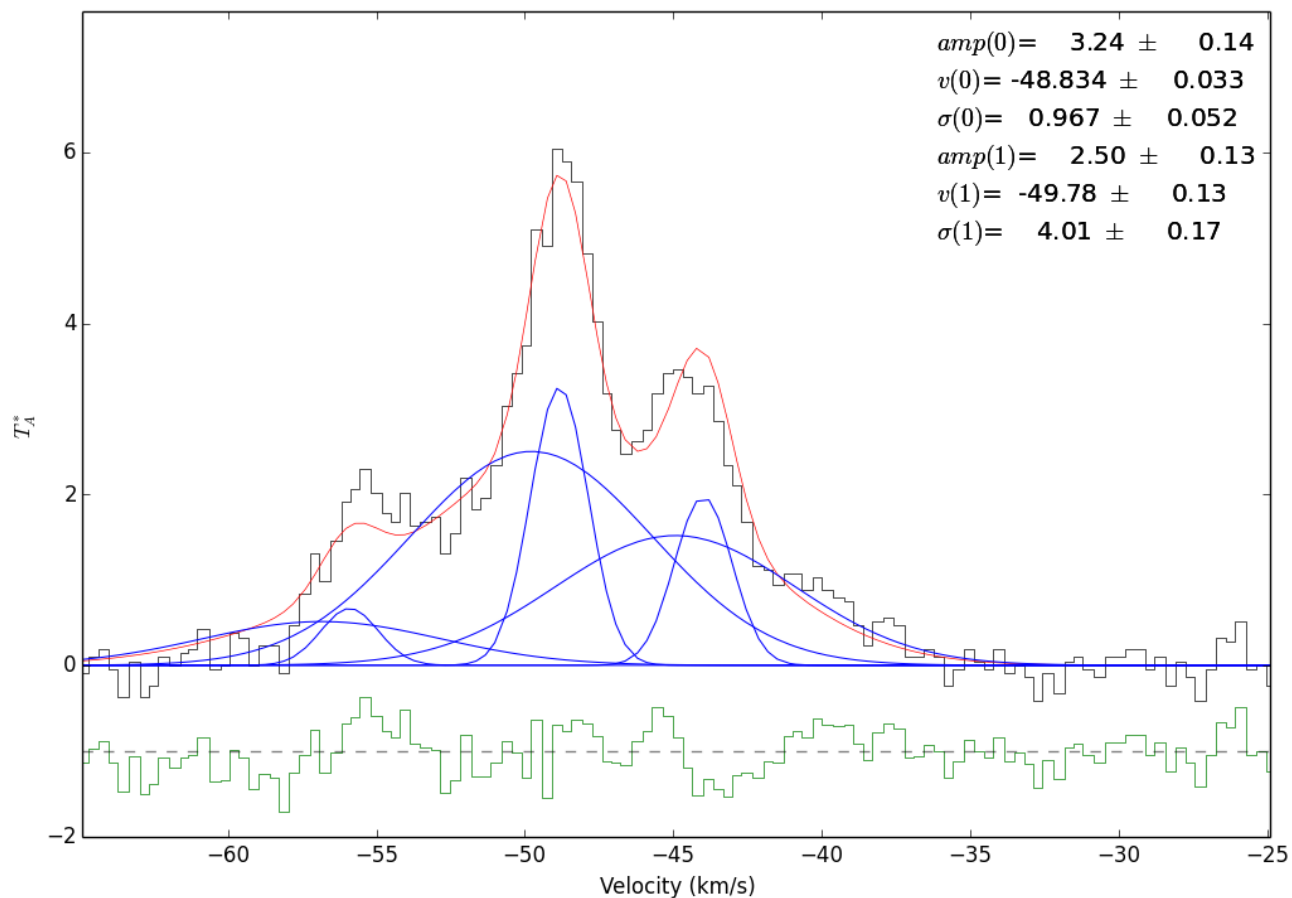


Fig. 12: A two-component fit to the same spectrum. It appears to be a much better fit, hinting that there are indeed two components (though the fit is probably not unique)

(continued from previous page)

```

# Note that the errors on the fits are larger than the fitted parameters.
# That's because this spectrum did not have an error assigned to it.
# Let's use the residuals:
spec.specfit.plotresiduals()

# Now, refit with error determined from the residuals:
# (we pass in guesses to save time / make sure nothing changes)
spec.specfit(guesses=spec.specfit.modelpars)

# Save the figures to put on the web...
spec.plotter.figure.savefig("simple_fit_example_HCOp.png")
spec.specfit.residualaxis.figure.savefig("simple_fit_example_HCOp_residuals.png")

# Also, let's crop out stuff we don't want...
spec.crop(-100,100)
# replot after cropping (crop doesn't auto-refresh)
spec.plotter()
# replot the fit without re-fitting
spec.specfit.plot_fit()
# show the annotations again
spec.specfit.annotate()

spec.plotter.figure.savefig("simple_fit_example_HCOp_cropped.png")

```

## 8.14 Fitting H2 1-0 S(1) line in NIR data cube

```

import astropy
import pyspeckit
import pylab as pl
import numpy as np
import astropy.io.fits as pyfits

# load the cube as a pyspeckit Cube
# I usually get an error here if cube.fits' header doesn't have 'CTYPE3' = 'WAVE'
cube = pyspeckit.Cube('cube.fits')

# Slice the cube over the wavelength range you'd like to fit
cube_h2 = cube.slice(21145,21250,unit='Angstrom')

# rescale data to make fitting nicer
# I add an offset to avoid negative values
cube_h2.cube *= 1e17
cube_h2.cube += 30.

# Do an initial plot & fit of a single spectrum
# at a pixel with good S/N
cube_h2.plot_spectrum(100,100)

#### The following command is just for setup! The actual fitting occurs below. ####
# Here I'm fitting two gaussians with 4 parameters each (background offset,
# amplitude, wavelength centroid, linewidth).
# I find that if I let both backgrounds be free parameters, pyspeckit returns
# unrealistic values for both backgrounds, so I fix the 2nd gaussian's background

```

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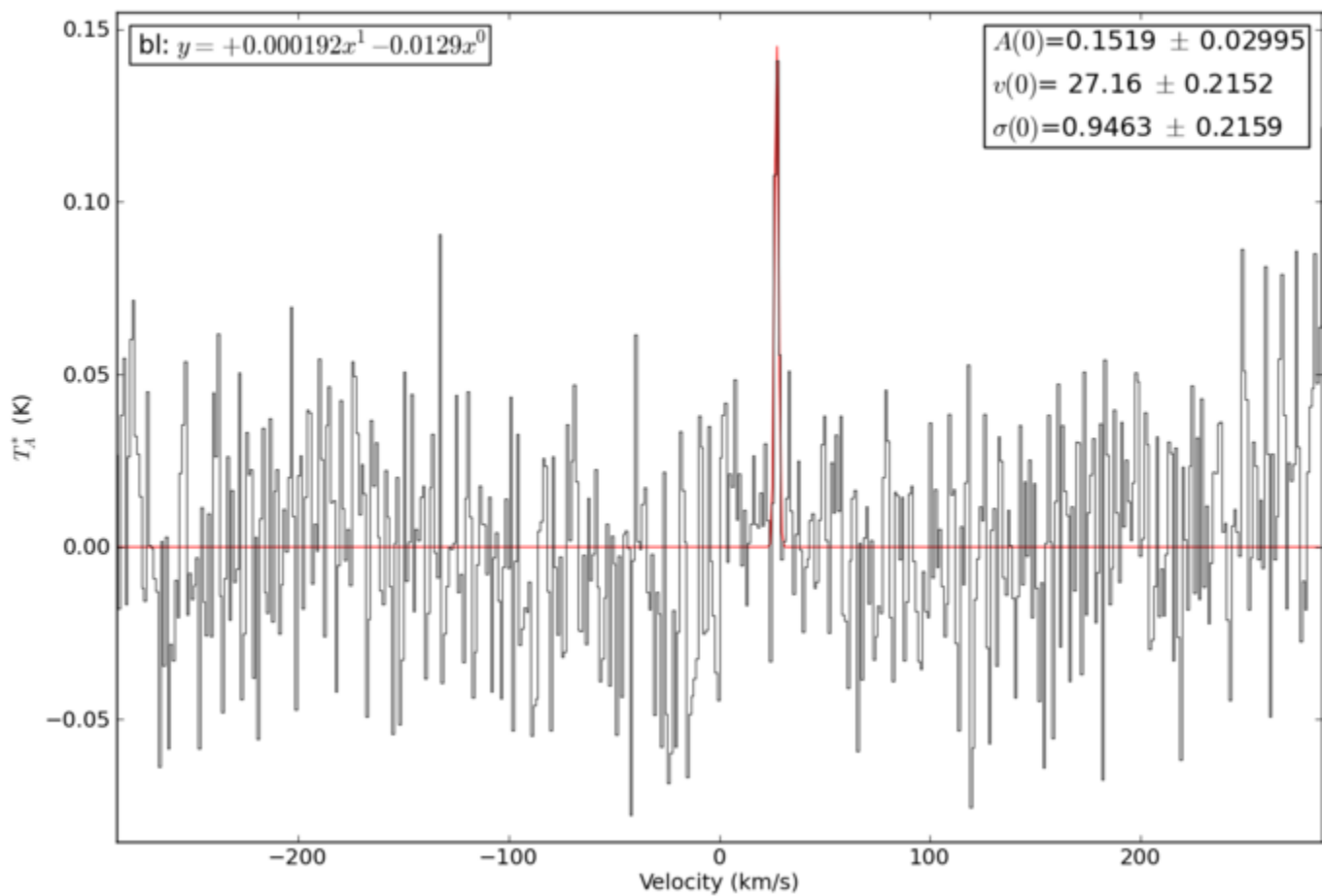


Fig. 13: Sample HCO+ spectrum fitted with a gaussian

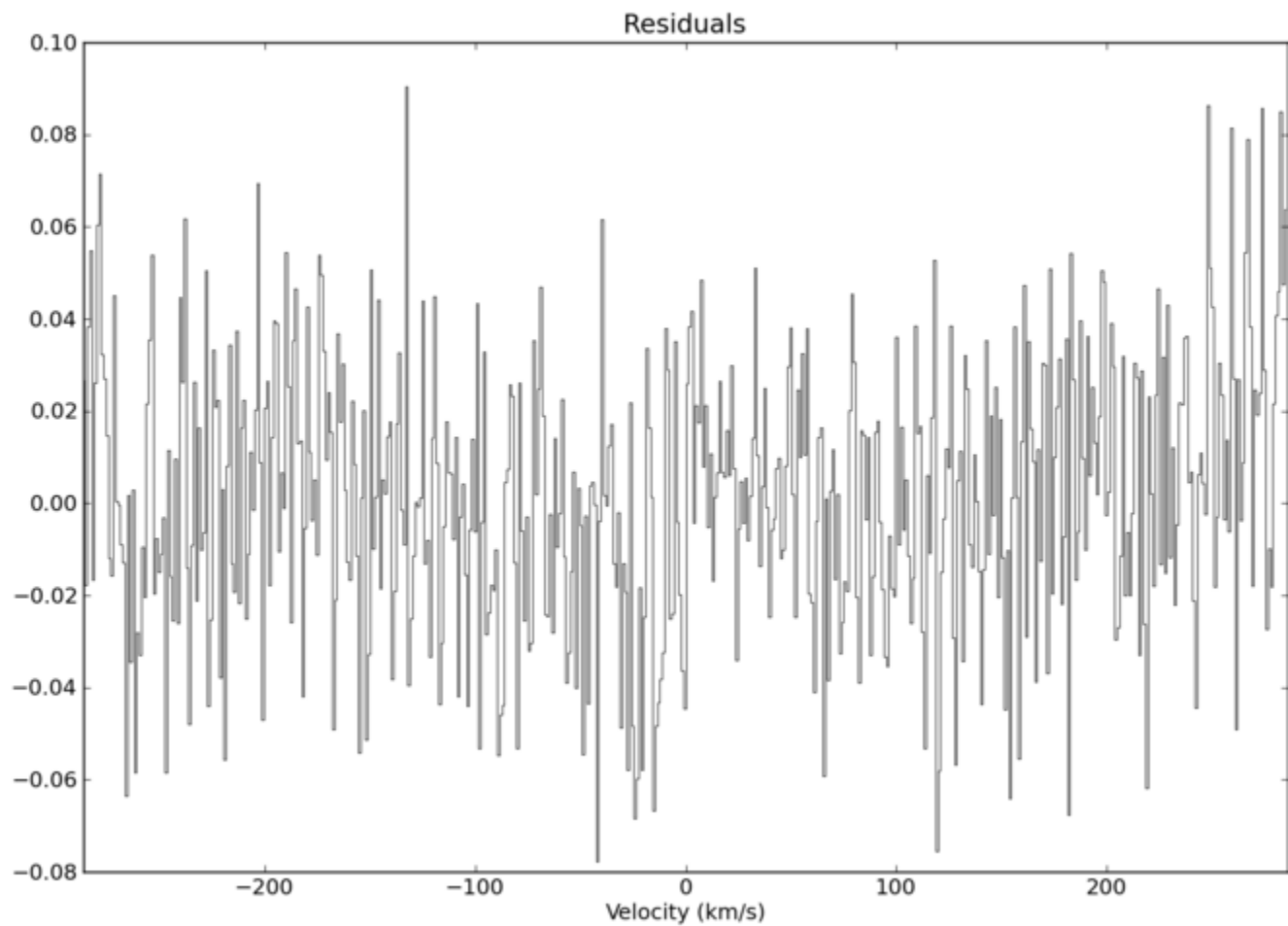


Fig. 14: Residuals of the gaussian fit from the previous figure

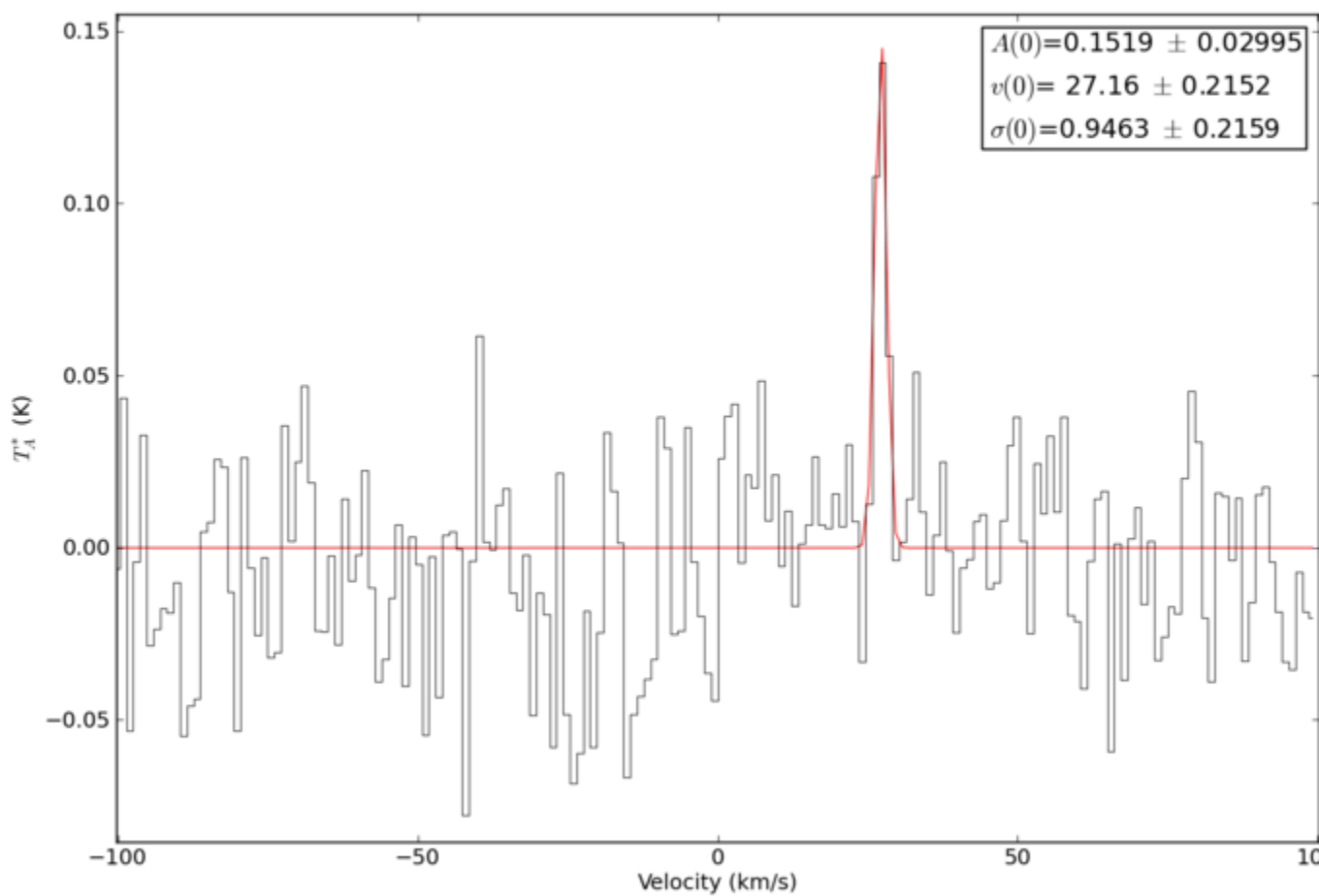


Fig. 15: A zoomed-in, cropped version of the spectrum. With the ‘crop’ command, the excess data is discarded.



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```

# level to 0. The actual command to fix the parameter comes in the fiteach call.
cube_h2.specfit(fittype='vheightgaussian',guesses=[3,1,2.1220e4,2,0,50,21232.,2],quiet=False,save=False)

# Get ready for the interactive plots that come up after fiteach finishes
cube_h2.mapplot.makeplane(estimator=np.nansum)

# For my cube.fits, (21145,21195) covers a part of the spectrum that is free of
# spectral lines. The std variable will be used to estimate the S/N of a line
# during fiteach.
std = cube_h2.stats((21145,21195))['std']

#### Here's where all the fitting happens.
## With the "parlimited" and "parlimits" keywords, I have restricted
## the range for the wavelength centroid and linewidth parameters.
## With the "fixed" keyword, I have held the 2nd gaussian's background level
## to zero, and the "signal_cut" keyword rejects fits for voxels below a
## user-specified S/N threshold.
cube_h2.fiteach(use_nearest_as_guess=False,
               guesses=[3,1,2.1220e4,2,0,50,21232.,2],
               fittype='vheightgaussian',
               integral=False,
               multicore=4,
               negamp=False,
               verbose_level=2,
               errspec=np.ones(cube_h2.shape)*std,
               parlimited=[(False,False), (False,False), (True,True),
                          (True,True), (False,False), (True,True),
                          (True,True), (True,True)],
               parlimits=[(0.9,1.4), (0,16), (21210,21225), (0.5,5),
                          (0.9,1.4), (0,100), (21227.,21236), (0.5,5)],
               fixed=[False, False, False, False, True, False, False,
                      False],
               signal_cut=20,
               start_from_point=(100,100))

# plot the fits as images (you can click on background image to see the spectra + fits)
amp_max = np.max(cube_h2.parcube[1,:,:])
cube_h2.mapplot(estimator=1,vmax=amp_max,vmin=0)
cube_h2.mapplot.axis.set_title("Amplitude")

cube_h2.mapplot.figure=pl.figure(5)
cube_h2.mapplot(estimator=3, vmax=5, vmin=0)
cube_h2.mapplot.axis.set_title("Line Width")

cube_h2.mapplot.figure=pl.figure(6)
cube_h2.mapplot(estimator=2,vmin=21215,vmax=21225)
cube_h2.mapplot.axis.set_title("Line Center")

cube_h2.mapplot.figure=pl.figure(7)
cube_h2.mapplot(estimator=0,vmax=100,vmin=0)
cube_h2.mapplot.axis.set_title("Background")
pl.show()

## Create the image
background = (cube_h2.parcube[0,:,:] - 30.) / 1e17
amplitude = cube_h2.parcube[1,:,:] / 1e17
linecenter = cube_h2.parcube[2,:,:]

```

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```

sigma = cube_h2.parcube[3,:,:] / 3e5 * h2_linecenter
image = np.sqrt(2*np.pi)*h2_amplitude*h2_sigma

# Clean up the header
# (this is a bit of a hacky way to do it, but it works)
cube_h2.header['NAXIS'] = 2
del cube_h2.header['NAXIS3']
# a nicer way is to use WCS:
from astropy import wcs
newheader = wcs.WCS(cube_h2.header).sub([wcs.WCSSUB_CELESTIAL]).to_header()
cube2.header = newheader
# however, this approach may lose other important header keywords

# Write the image to file
h2filename = input_filename.replace("cube.fits", "h2_1-0S1.fits")
h2fits = pyfits.PrimaryHDU(data=h2_image, header=cube_h2.header)
if astropy.version.major >= 2 or (astropy.version.major==1 and astropy.version.minor>=3):
    h2fits.writeto(h2filename, overwrite=True)
else:
    h2fits.writeto(h2filename, clobber=True)

# Write pyspeckit parcube and errcube to file
pyspeckit_fits_filename = input_filename.replace("cube.fits",
                                                  "pyspeckitfits_h2_1-0S1.fits")
cube_h2.write_fit(pyspeckit_fits_filename, overwrite=True)

```

## 8.15 Optical fitting: The H $\alpha$ -[NII] complex of a type-I Seyfert galaxy

Source file for this example is here: [https://github.com/pyspeckit/pyspeckit/blob/master/examples/sn\\_example.py](https://github.com/pyspeckit/pyspeckit/blob/master/examples/sn_example.py)

```

import pyspeckit

# Rest wavelengths of the lines we are fitting - use as initial guesses
NIIa = 6549.86
NIIb = 6585.27
Halpha = 6564.614
SIIa = 6718.29
SIIb = 6732.68

# Initialize spectrum object and plot region surrounding Halpha-[NII] complex
spec = pyspeckit.Spectrum('sample_sdss.txt', errorcol=2)
spec.plotter(xmin = 6450, xmax = 6775, ymin = 0, ymax = 150)

# We fit the [NII] and [SII] doublets, and allow two components for Halpha.
# The widths of all narrow lines are tied to the widths of [SII].
guesses = [50, NIIa, 5, 100, Halpha, 5, 50, Halpha, 50, 50, NIIb, 5, 20, SIIa,
           5, 20, SIIb, 5]
tied = ['', '', 'p[17]', '', '', 'p[17]', '', 'p[4]', '', '3 * p[0]', '',
        'p[17]', '', '', 'p[17]', '', '', '']

# Actually do the fit.
spec.specfit(guesses = guesses, tied = tied, annotate = False)
spec.plotter.refresh()

```

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```

# Let's use the measurements class to derive information about the emission
# lines. The galaxy's redshift and the flux normalization of the spectrum
# must be supplied to convert measured fluxes to line luminosities. If the
# spectrum we loaded in FITS format, 'BUNITS' would be read and we would not
# need to supply 'fluxnorm'.
spec.measure(z = 0.05, fluxnorm = 1e-17)

# Now overplot positions of lines and annotate

y = spec.plotter.ymax * 0.85    # Location of annotations in y

for i, line in enumerate(spec.measurements.lines.keys()):

    # If this line is not in our database of lines, don't try to annotate it
    if line not in spec.speclines.optical.lines.keys(): continue

    x = spec.measurements.lines[line]['modelpars'][1]    # Location of the emission line
    # Draw dashed line to mark its position
    spec.plotter.axis.plot([x]*2, [spec.plotter.ymin, spec.plotter.ymax],
                           ls='--', color='k')

    # Label it
    spec.plotter.axis.annotate(spec.speclines.optical.lines[line][-1], (x, y),
                               rotation = 90, ha = 'right', va = 'center')

# Make some nice axis labels
spec.plotter.axis.set_xlabel(r'Wavelength $(\AA)$')
spec.plotter.axis.set_ylabel(r'Flux  $10^{-17}$   $\mathrm{erg/s/cm^2/\AA}$ ')
spec.plotter.refresh()

# Print out spectral line information
print("Line   Flux (erg/s/cm^2)   Amplitude (erg/s/cm^2)"
      "      FWHM (Angstrom)   Luminosity (erg/s)")
for line in spec.measurements.lines.keys():
    print(line, spec.measurements.lines[line]['flux'],
          spec.measurements.lines[line]['amp'],
          spec.measurements.lines[line]['fwhm'],
          spec.measurements.lines[line]['lum'])

# Had we not supplied the objects redshift (or distance), the line
# luminosities would not have been measured, but integrated fluxes would
# still be derived. Also, the measurements class separates the broad and
# narrow H-alpha components, and identifies which lines are which. How nice!

spec.specfit.plot_fit()

# Save the figure
spec.plotter.figure.savefig("sdss_fit_example.png")

```

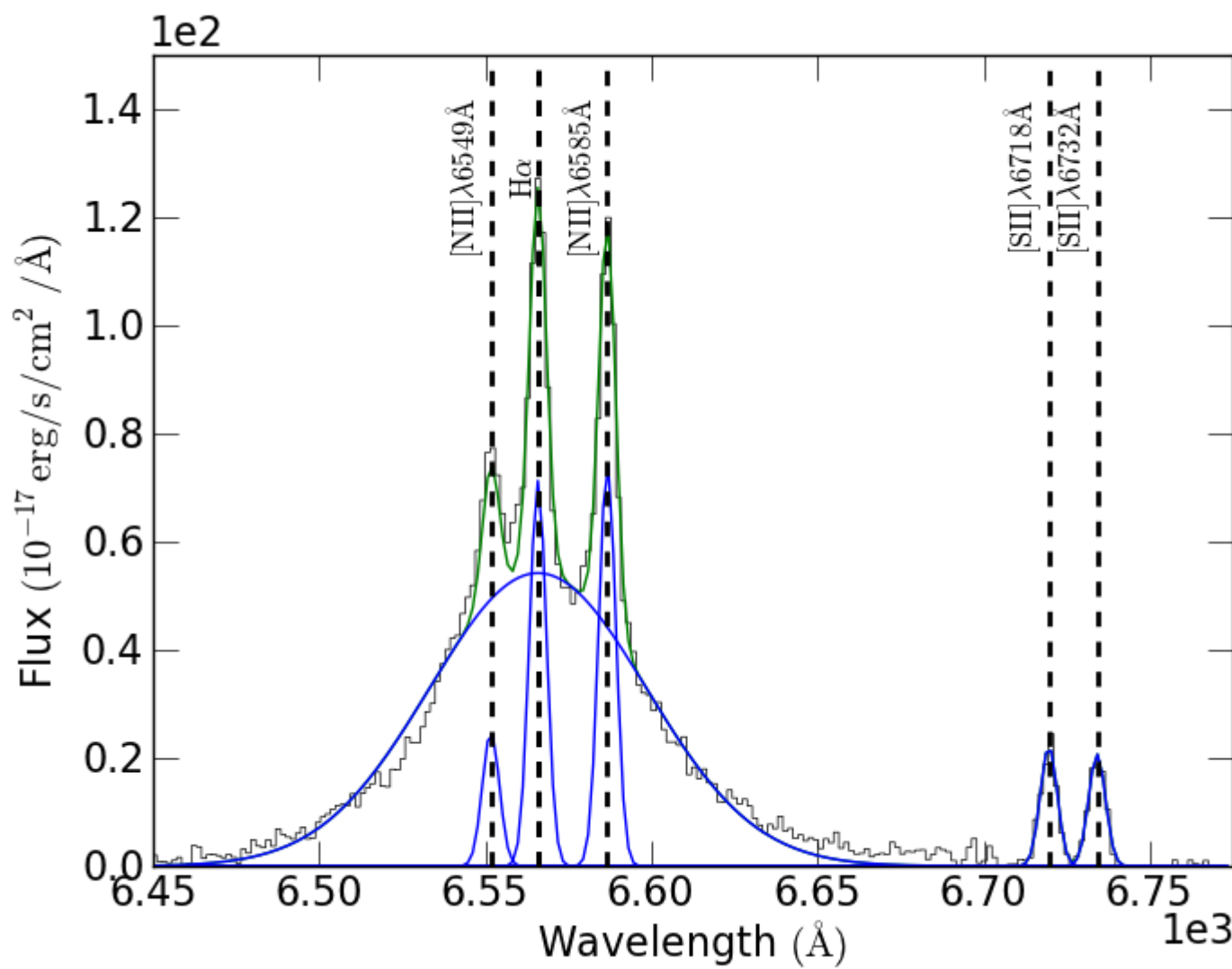
## 8.16 Optical Plotting - Echelle spectrum of Vega (in color!)

```

import pyspeckit
from pylab import *
import wav2rgb

```

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```

speclist = pyspeckit.wrappers.load_IRAF_multispec('evega.0039.rs.ec.dispcor.fits')

for spec in speclist:
    spec.units="Counts"

SP = pyspeckit.Spectra(speclist)
SPa = pyspeckit.Spectra(speclist,xunits='angstroms',quiet=False)

SP.plotter.figure=figure(1)
SPa.plotter.figure=figure(2)

figure(3)
clf()
figure(4)
clf()

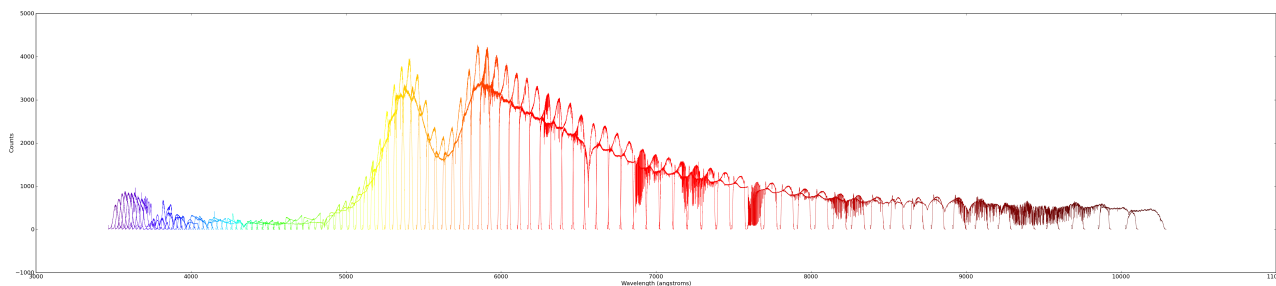
#clr = [list(clr) for clr in matplotlib.cm.brg(linspace(0,1,len(speclist)))]
clr = [wav2rgb.wav2RGB(c) + [1.0] for c in linspace(380,780,len(speclist))][::-1]
for ii,(color,spec) in enumerate(zip(clr,speclist)):
    spec.plotter.figure=figure(3), clear=False, reset=False, color=color, refresh=False)

    fig4=figure(4)
    fig4.subplots_adjust(hspace=0.35,top=0.97,bottom=0.03)
    spec.plotter(axis=subplot(10,1,ii%10+1), clear=False, reset=False, color=color, refresh=False)
    spec.plotter.axis.yaxis.set_major_locator( matplotlib.ticker.MaxNLocator(4) )

    if ii % 10 == 9:
        spec.plotter.refresh()
        spec.plotter.savefig('vega_subplots_%03i.png' % (ii/10+1))
        clf()

spec.plotter.refresh()

```



## 8.17 A guide to interactive fitting

A step-by-step example of how to use the interactive fitter.

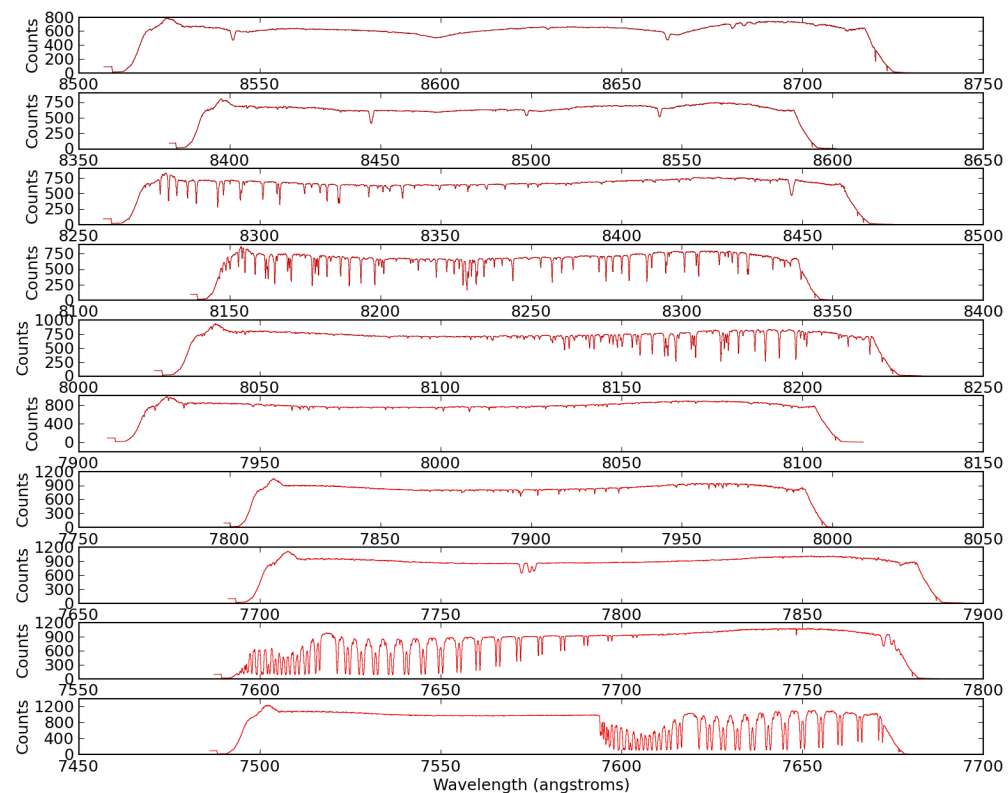
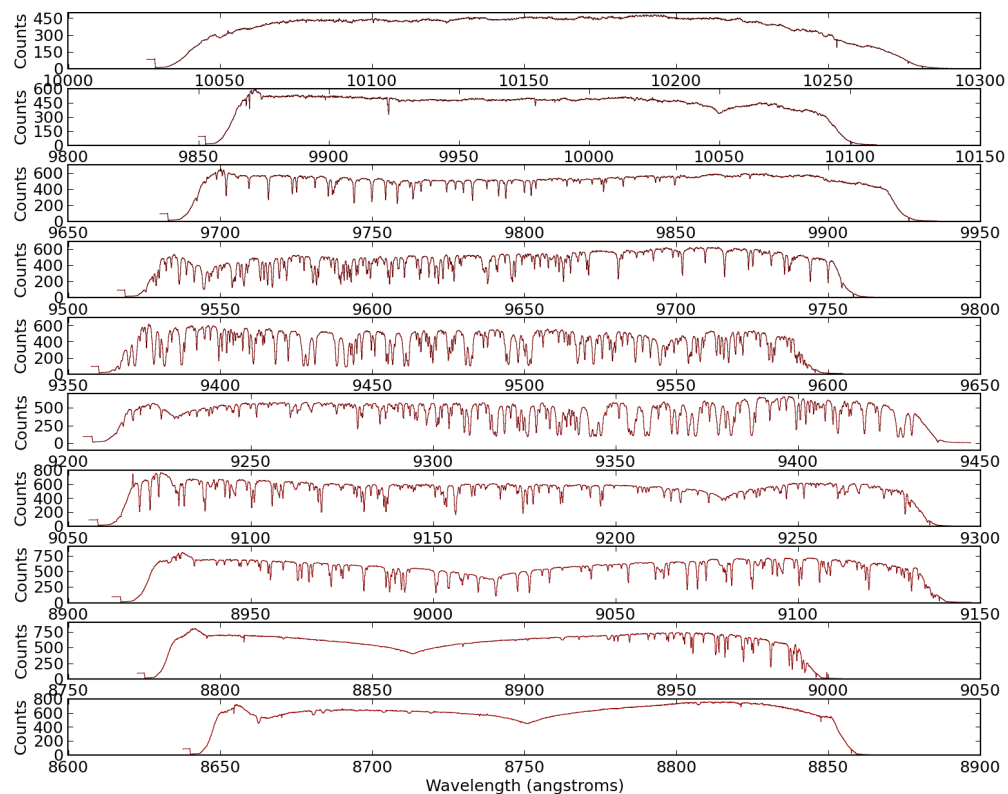
In short, we will do the following:

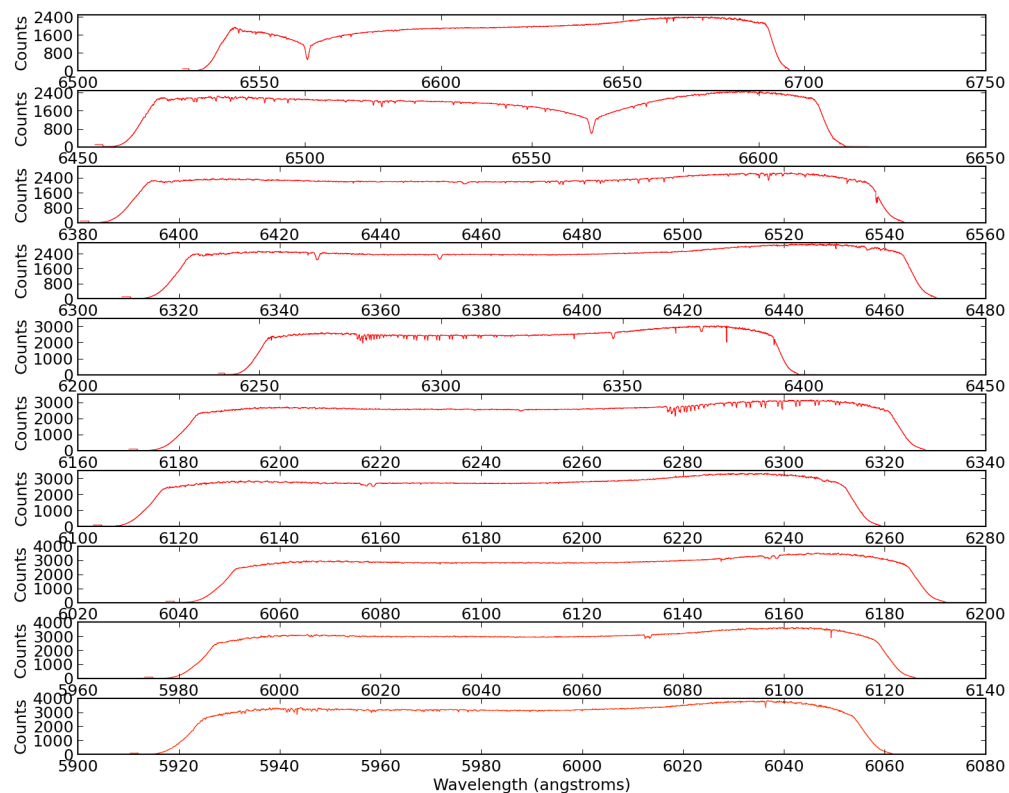
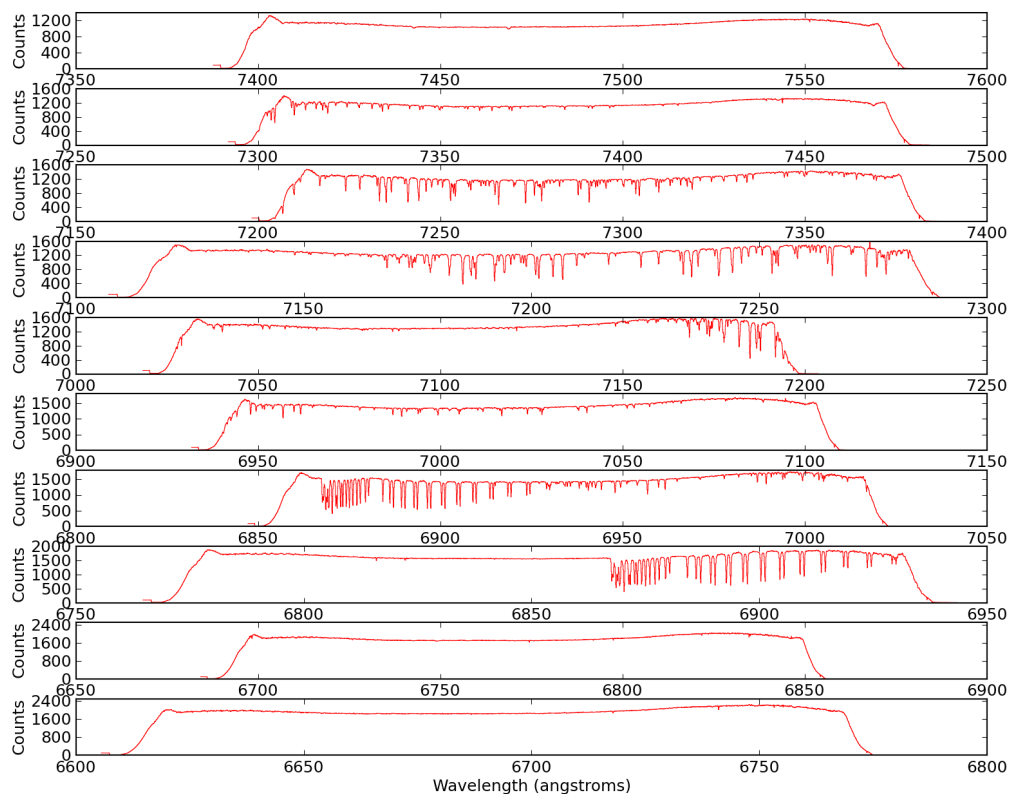
```

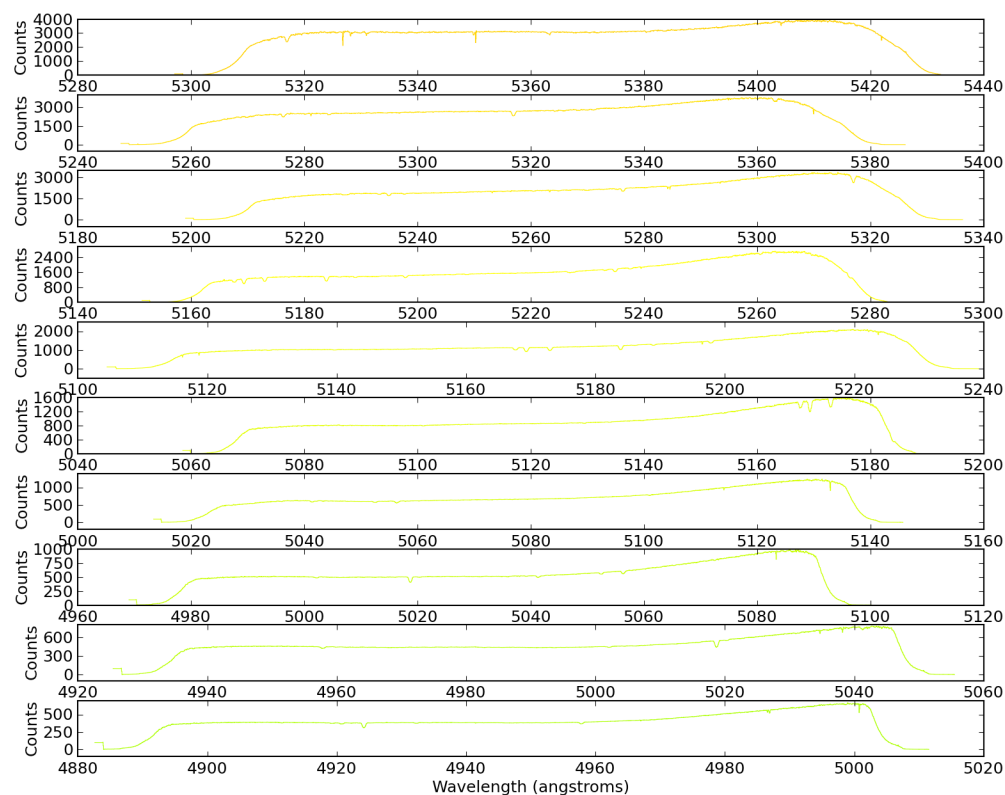
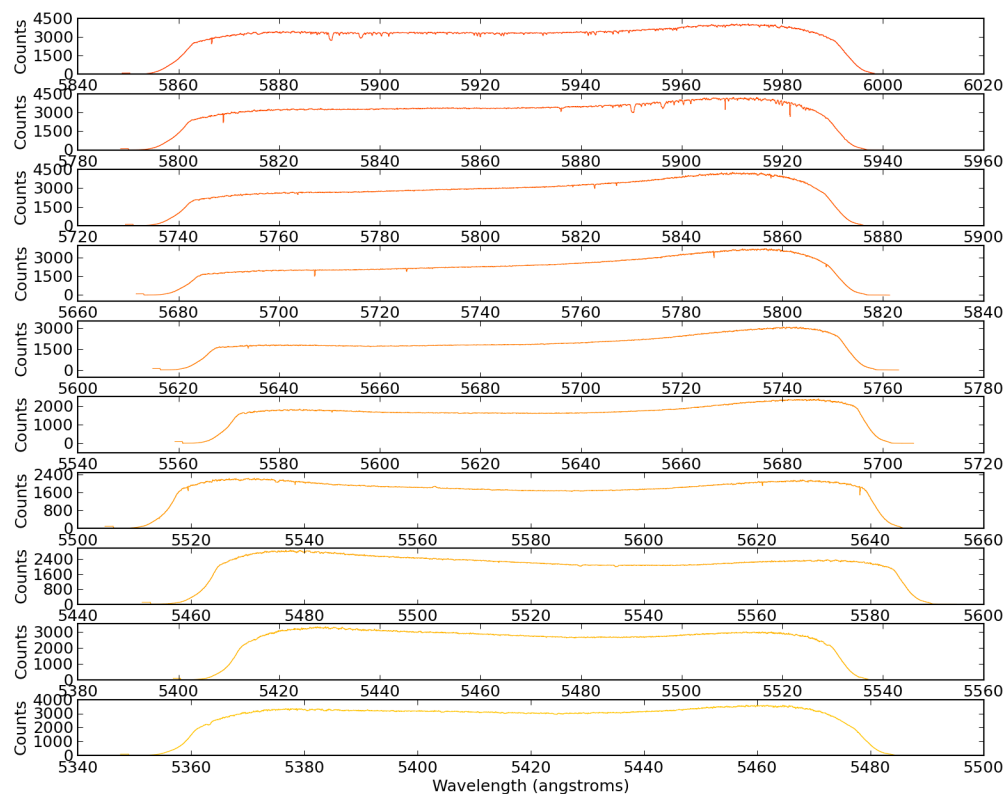
# 1. Load the spectrum
sp = pyspeckit.Spectrum('hr2421.fit')

```

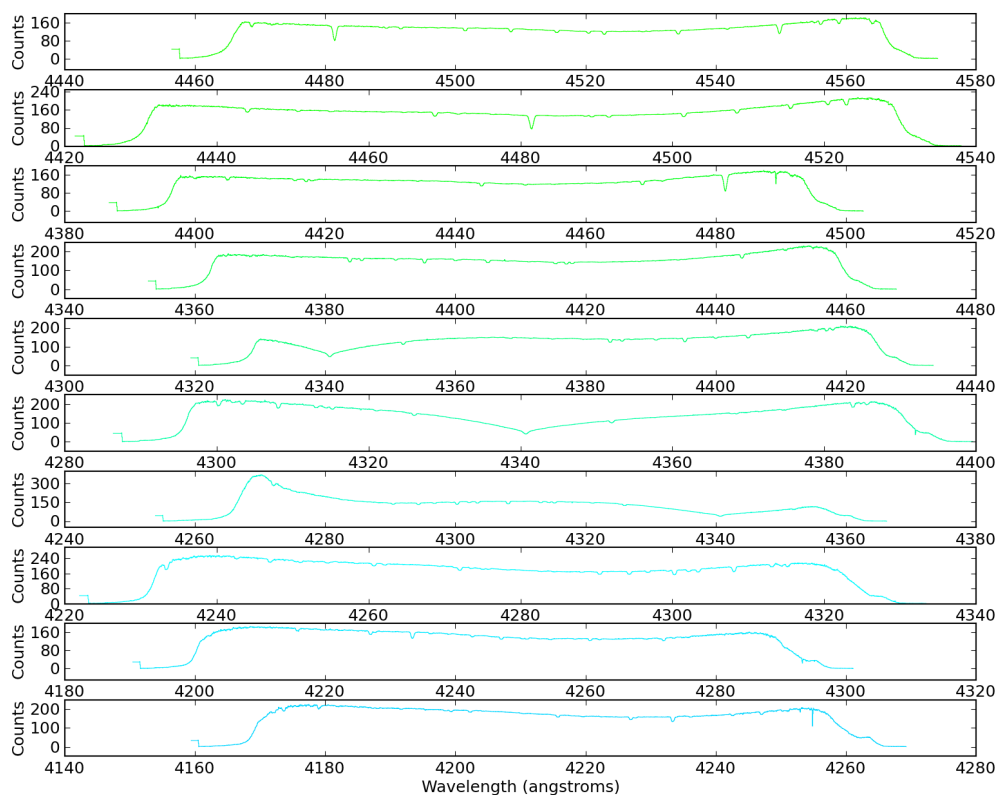
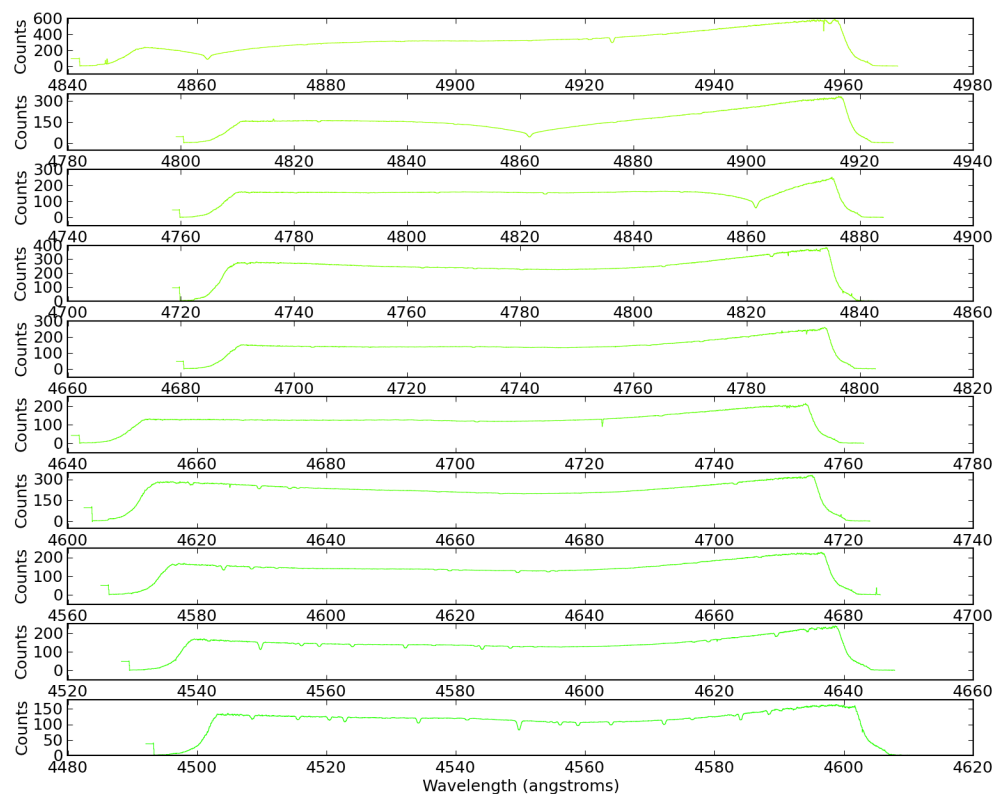
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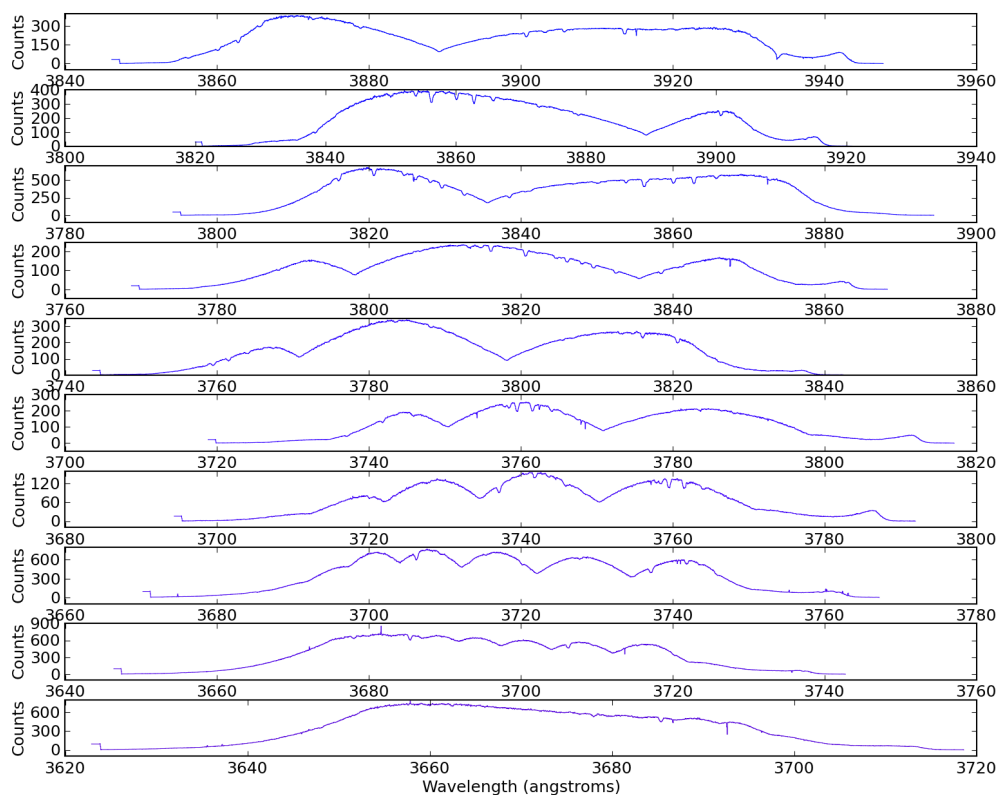
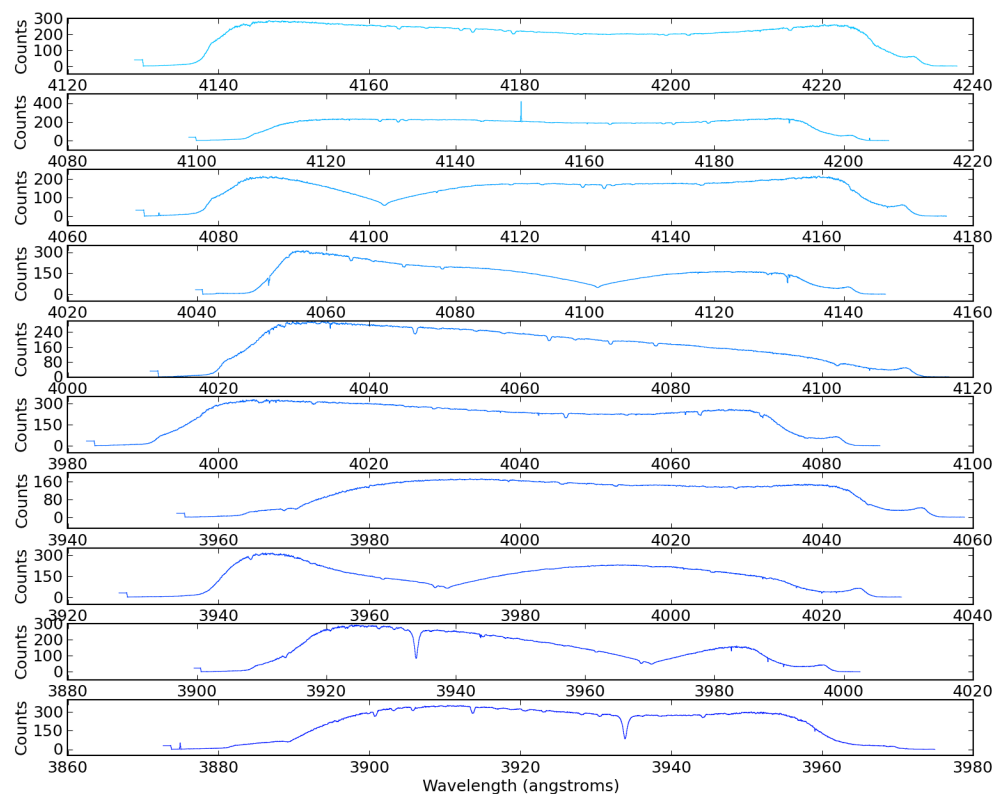












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```
# 2. Plot a particular spectral line
sp.plotter(xmin=4700,xmax=5000)

# 3. Need to fit the continuum first
sp.baseline(interactive=True, subtract=False)

# DO INTERACTIVE THINGS HERE
# 4... (much work takes place interactively at this stage)

# 5. Start up an interactive line-fitting session
# (do not run this line until *after* completing the baseline fitting)
#sp.specfit(interactive=True)
```

**Note:** If you don't see a plot window after step #2 above, make sure you're using matplotlib in interactive mode. This may require starting ipython as `ipython --pylab`

You can also start the interactive fitter by pressing 'b' for baseline or 'f' for fit when a plot window is active, then press '?' to get help. These commands will not work if you have the "zoom" or "pan" tools active, though!

This is where you start the line-fitter:

```
# Start up an interactive line-fitting session
sp.specfit(interactive=True)
```

## 8.18 Complicated H-alpha Line Fitting

Source code for this example

FITS file for this example

```
"""
Example demonstrating how to fit a complex H-alpha profile after
subtracting off a satellite line (in this case, He I 6678.151704)
"""
import pyspeckit

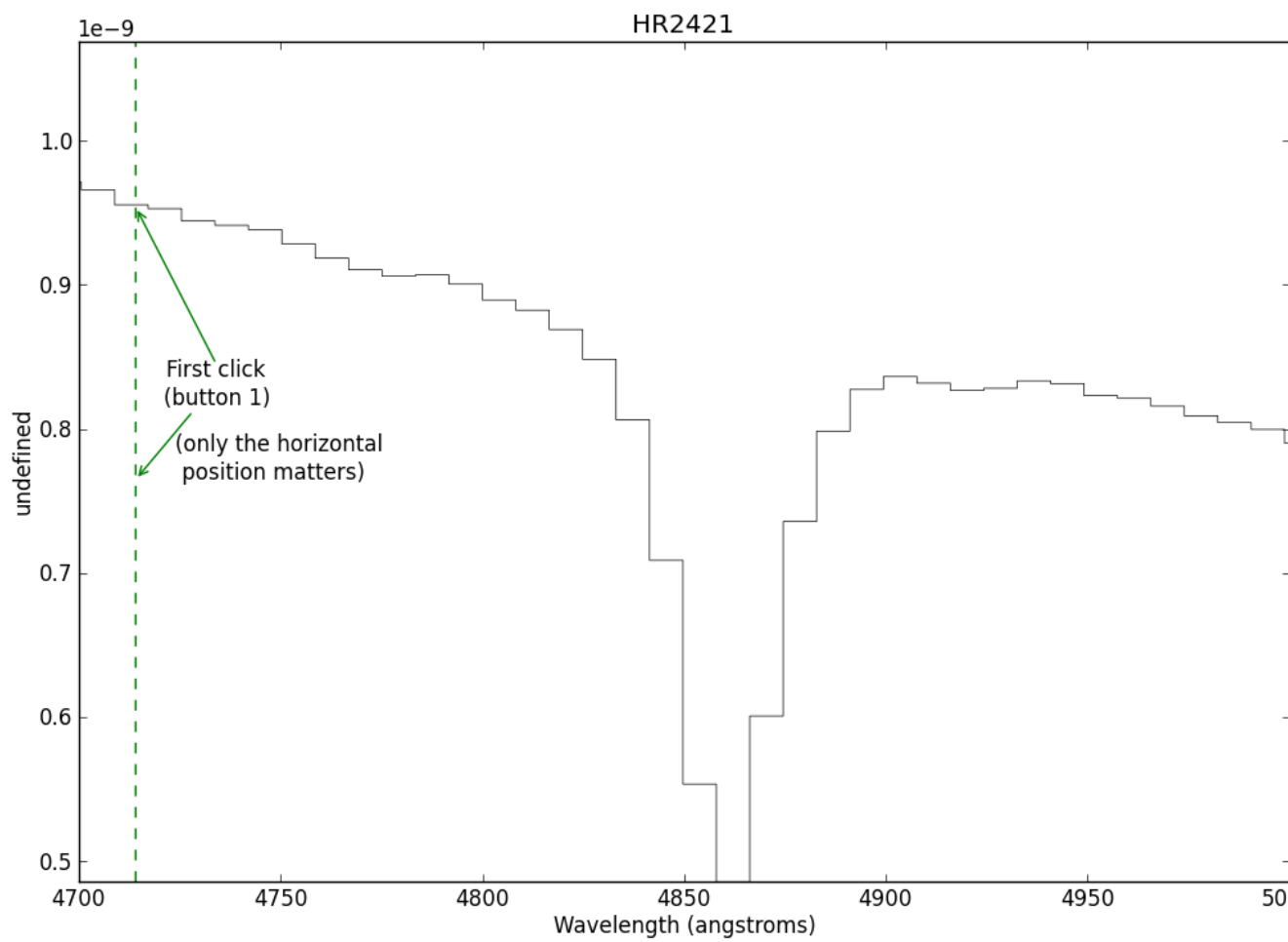
sp = pyspeckit.Spectrum('sn2009ip_halpha.fits')

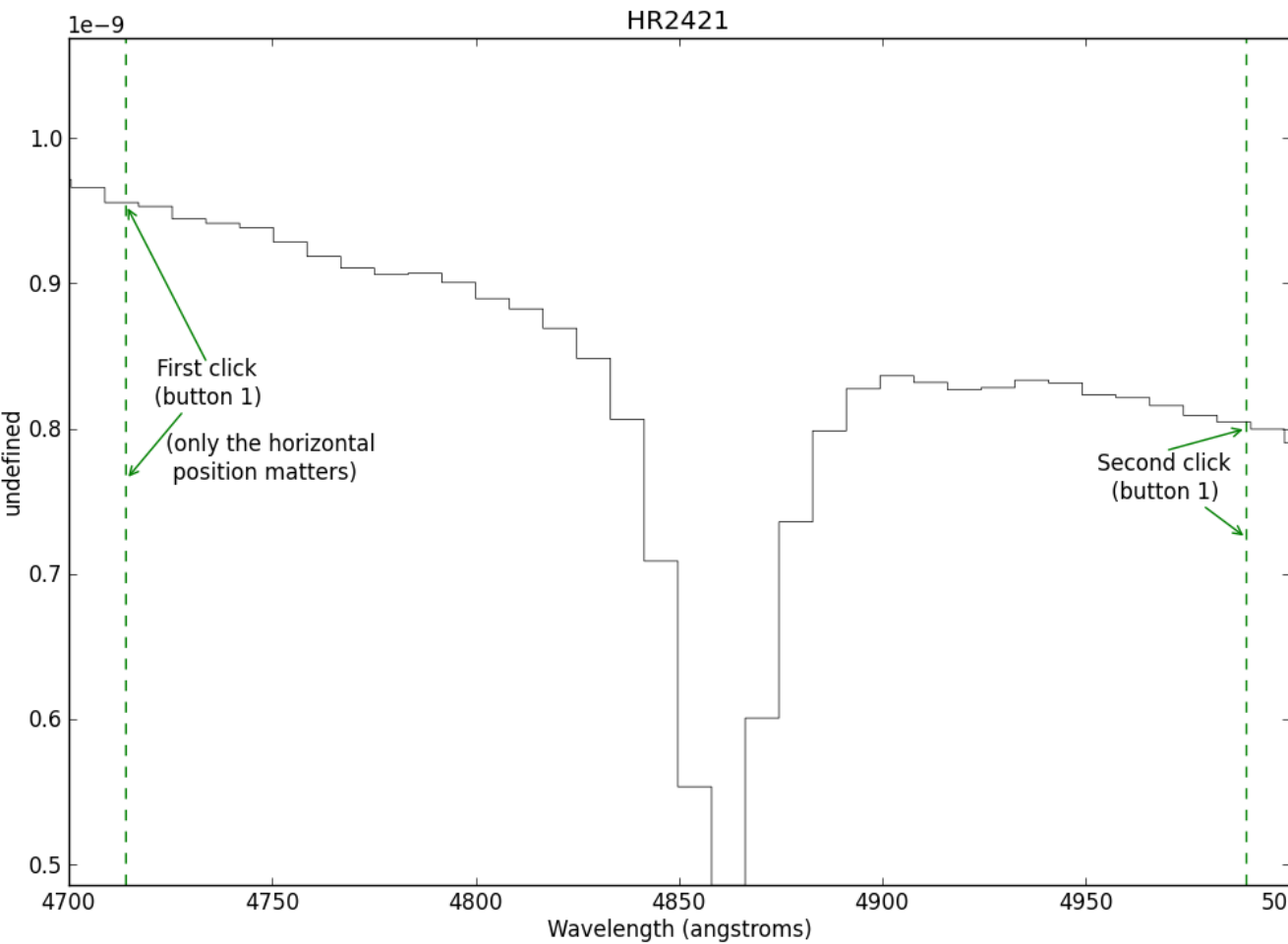
# start by plotting a small region around the H-alpha line
sp.plotter(xmin=6100,xmax=7000,ymax=2.23,ymin=0)

# the baseline (continuum) fit will be 2nd order, and excludes "bad"
# parts of the spectrum
# The exclusion zone was selected interactively
# (i.e., cursor hovering over the spectrum)
sp.baseline(xmin=6100, xmax=7000,
            exclude=[6450,6746,6815,6884,7003,7126,7506,7674,8142,8231],
            subtract=False, reset_selection=True, highlight_fitregion=True,
            order=2)

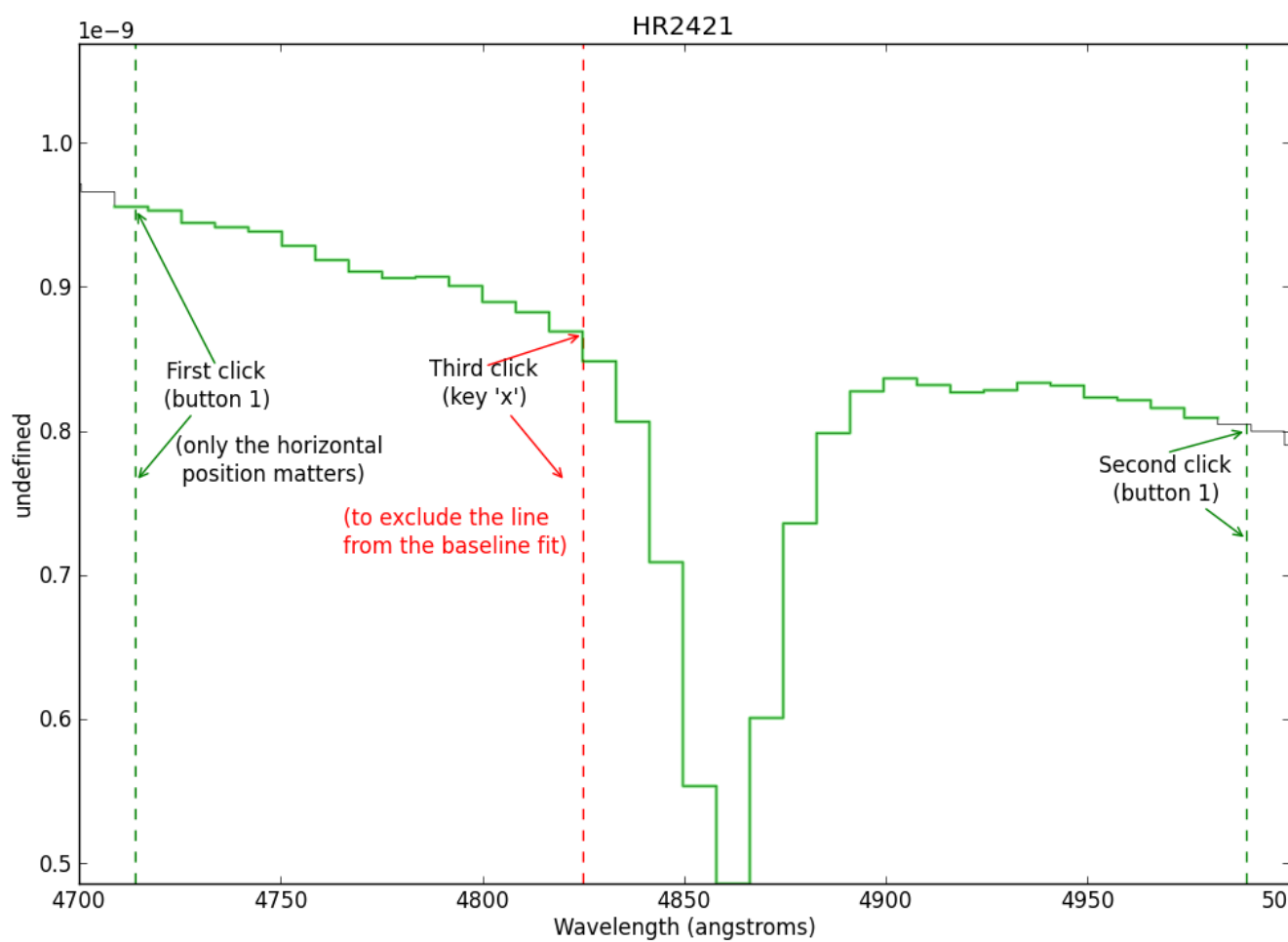
# Fit a 4-parameter voigt (figured out through a series of guess and check fits)
sp.specfit(guesses=[2.4007096541802202, 6563.2307968382256, 3.5653446153950314, 1,
                    0.53985149324131965, 6564.3460908526877, 19.443226155616617, 1,
```

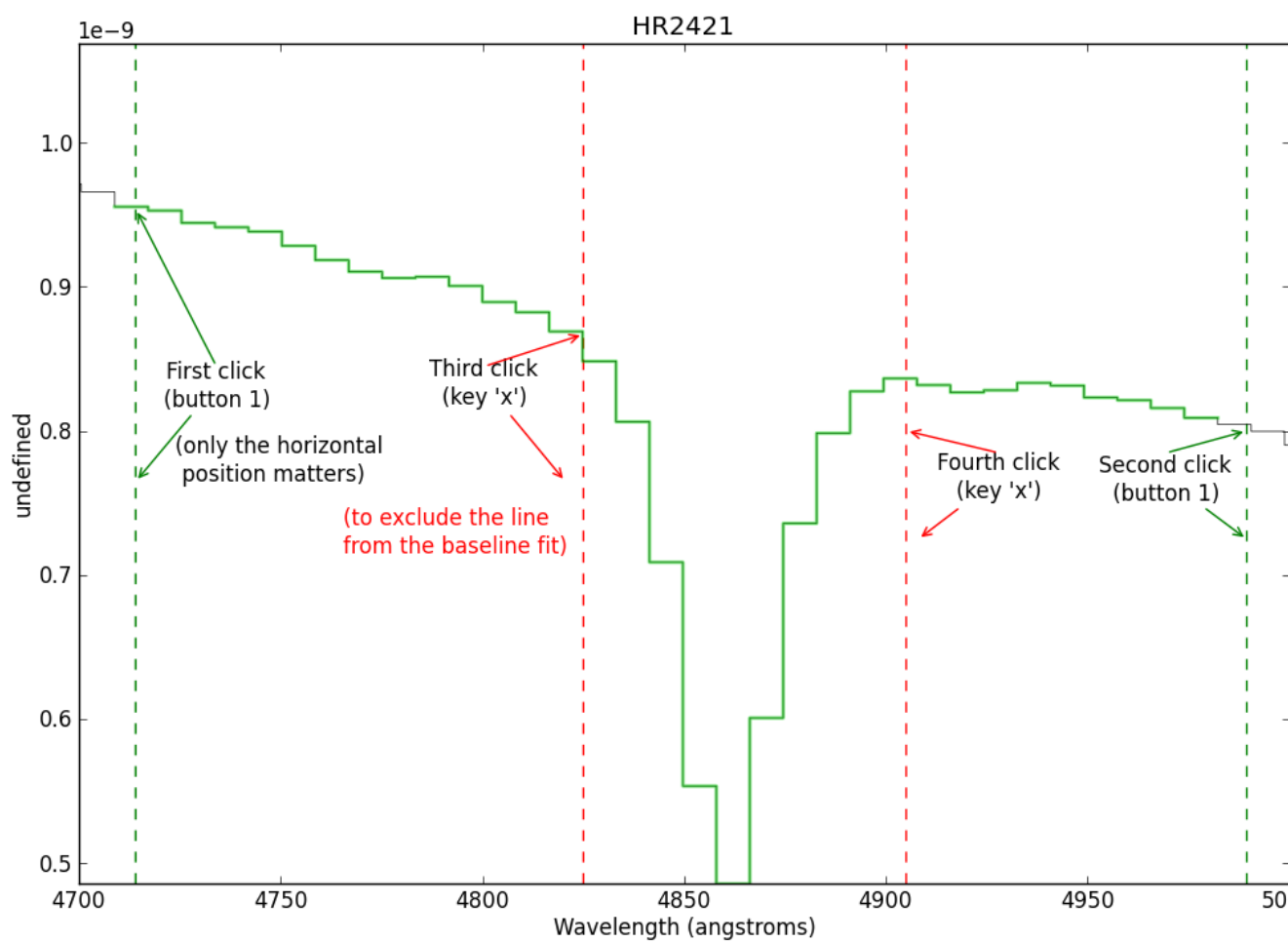
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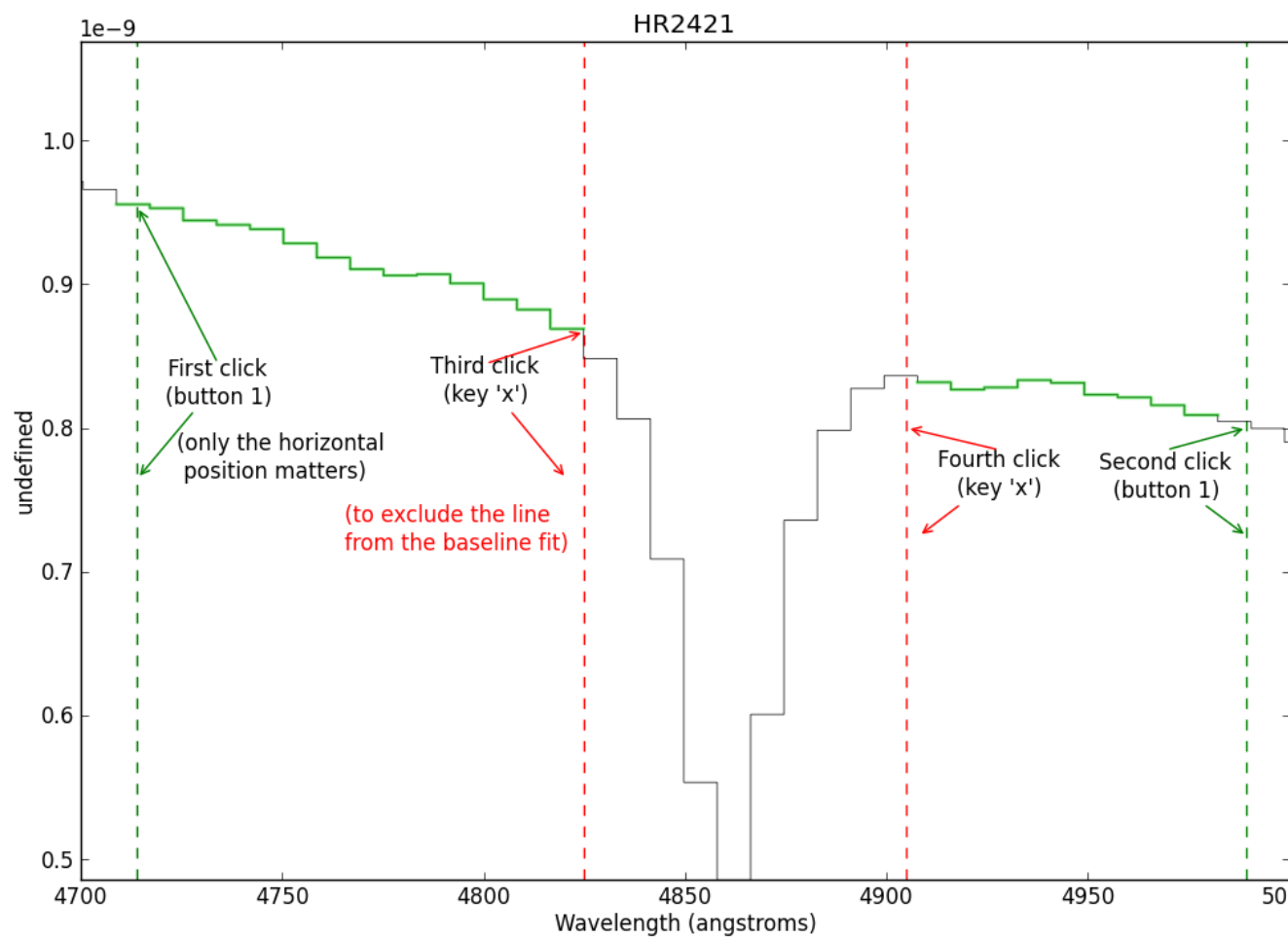


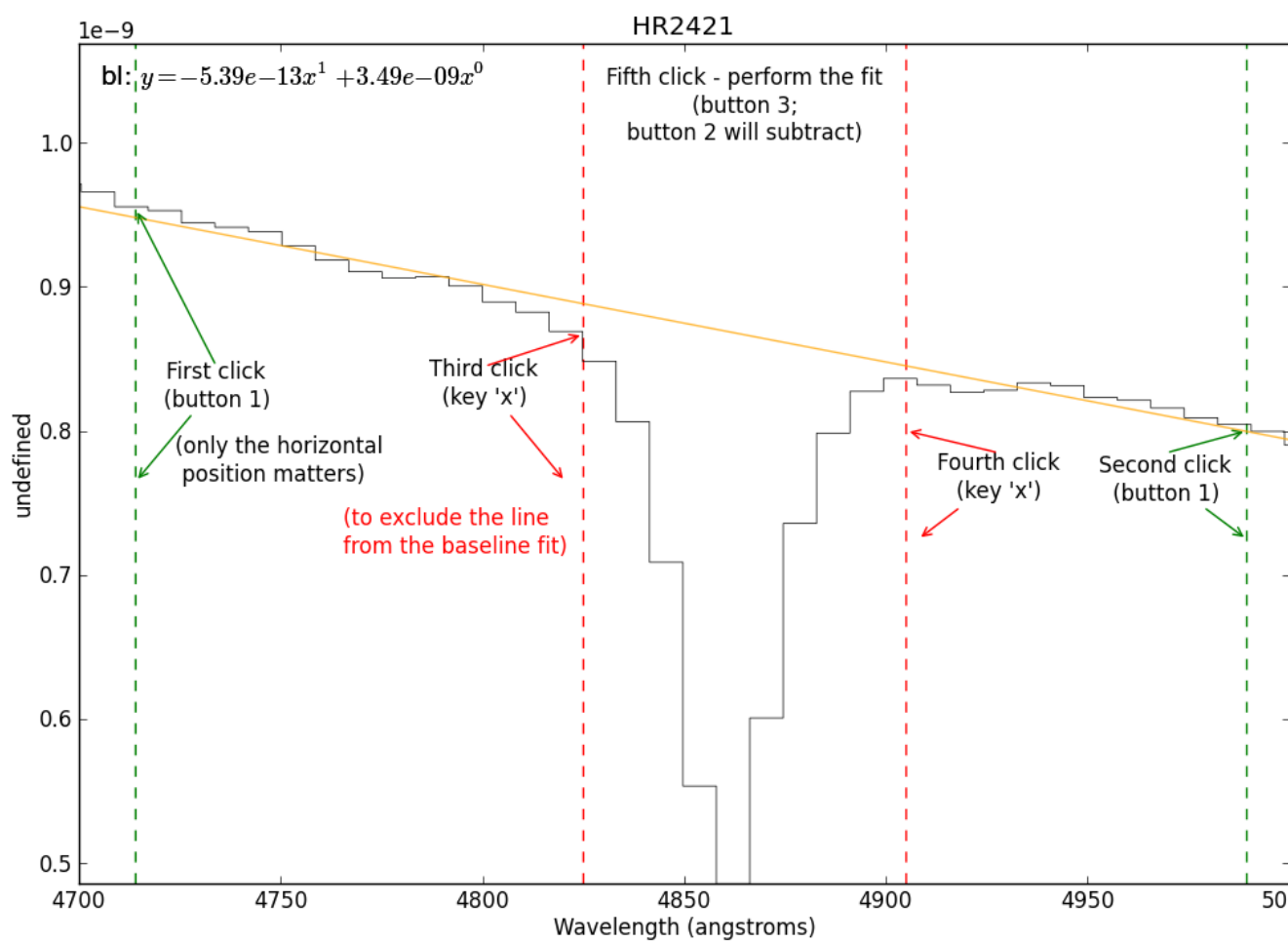


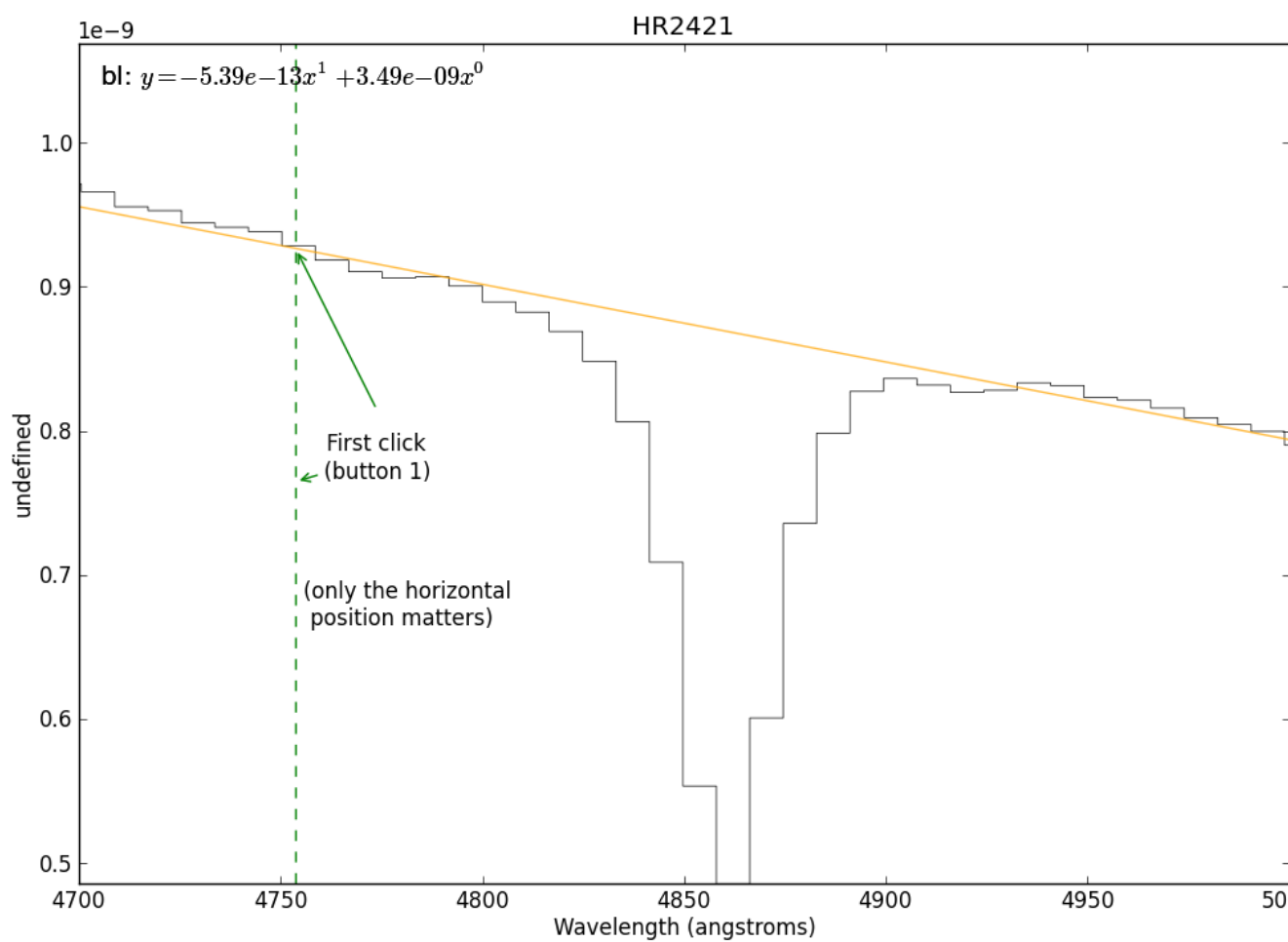


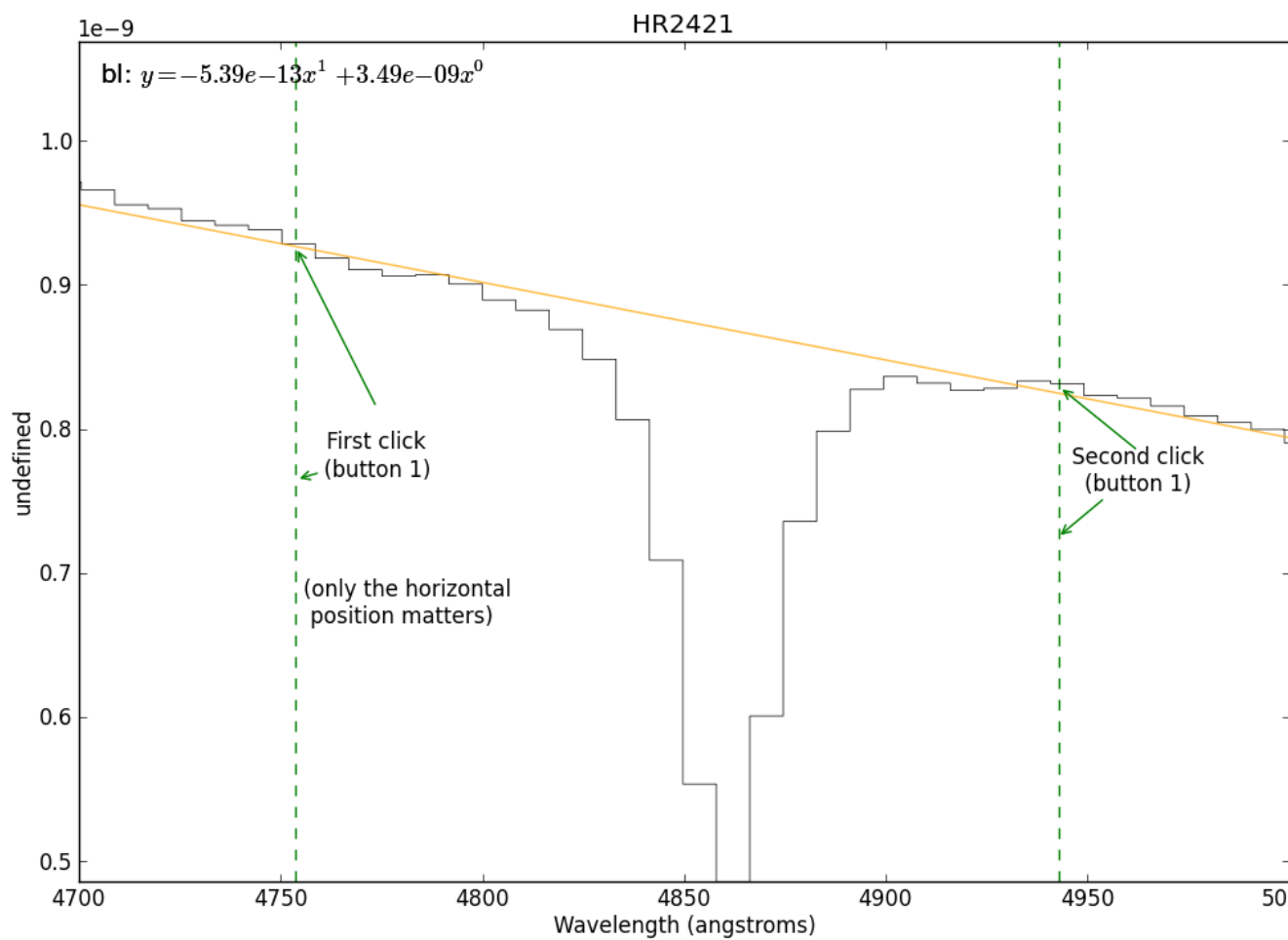


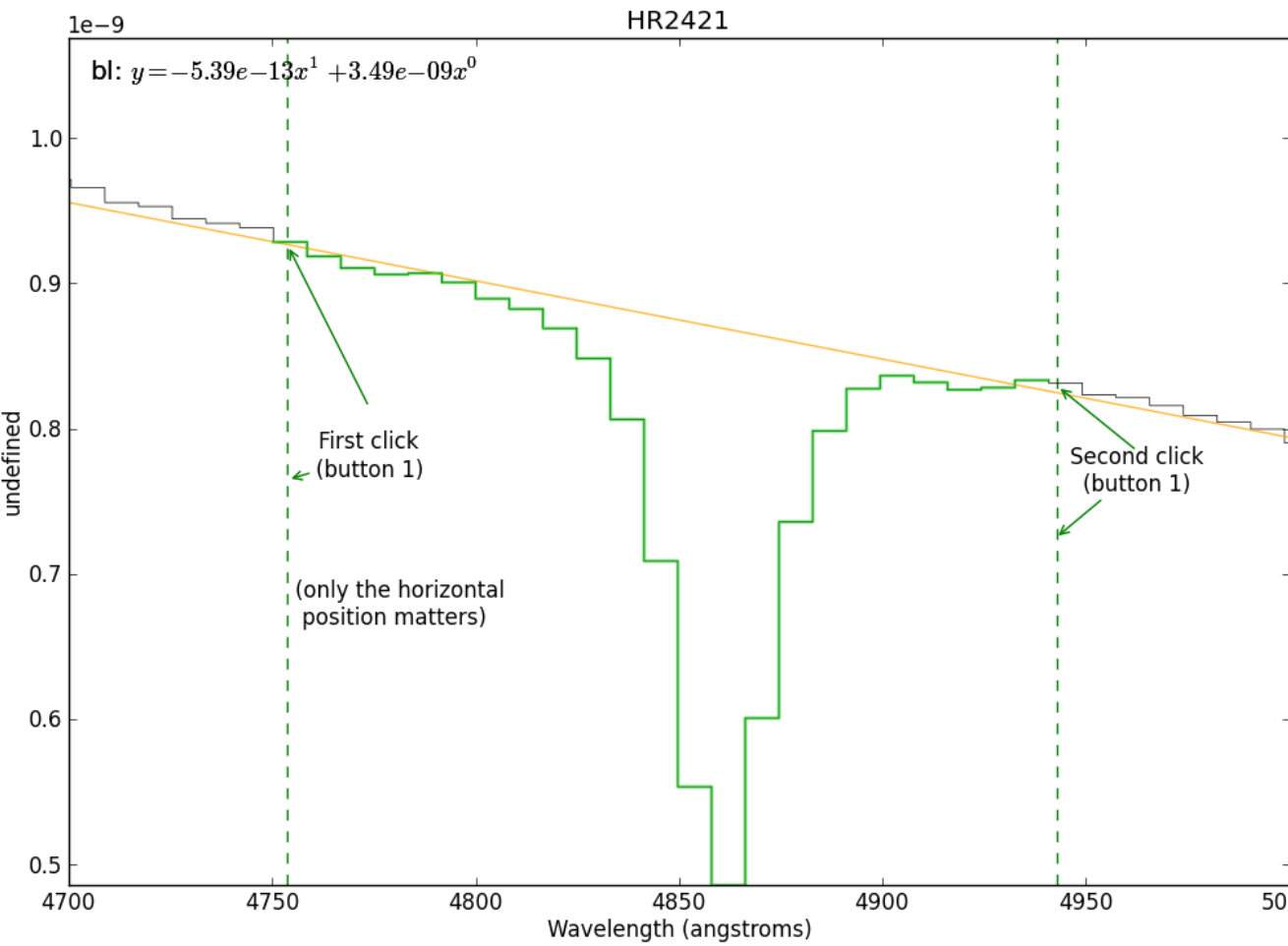


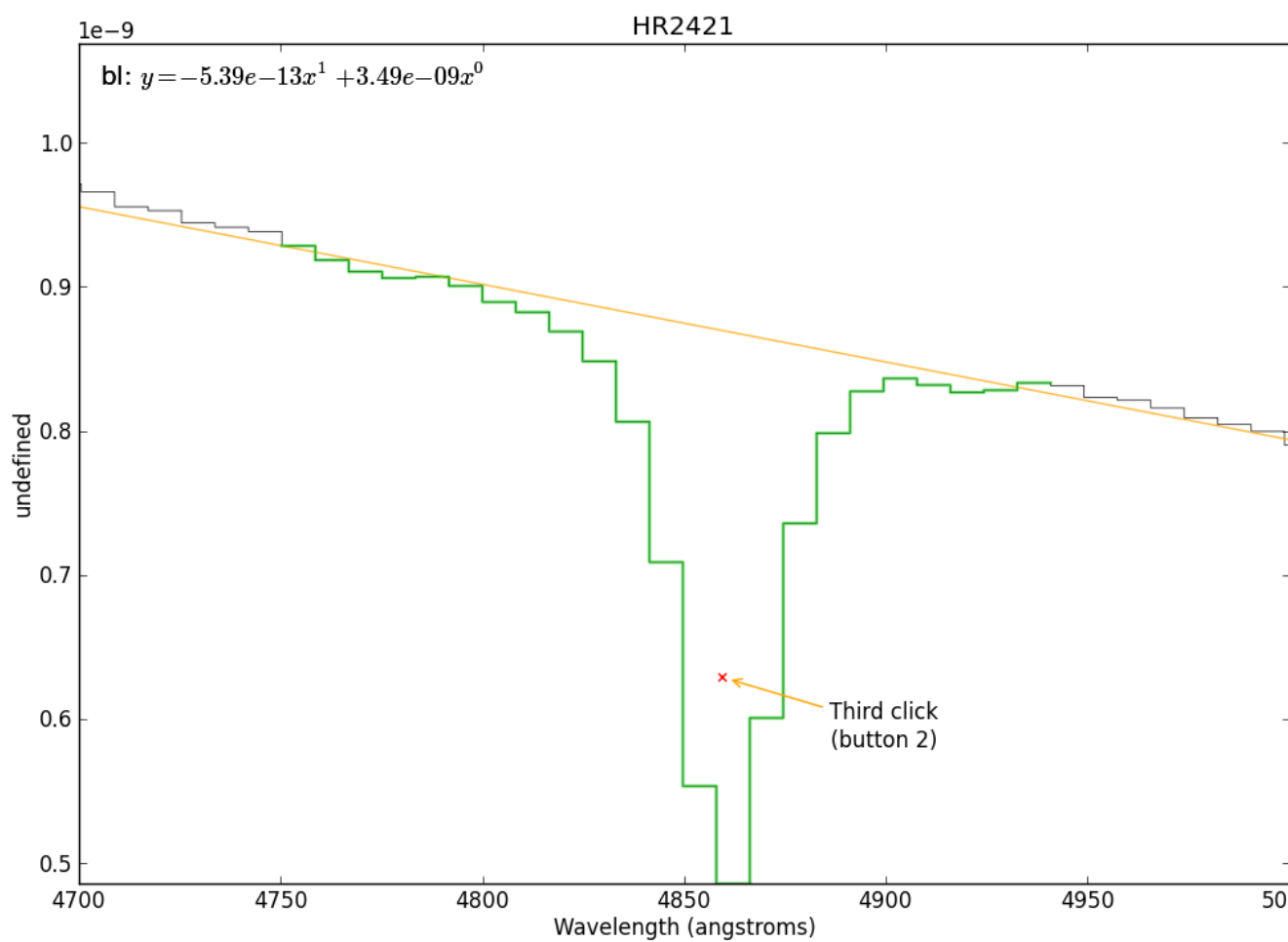


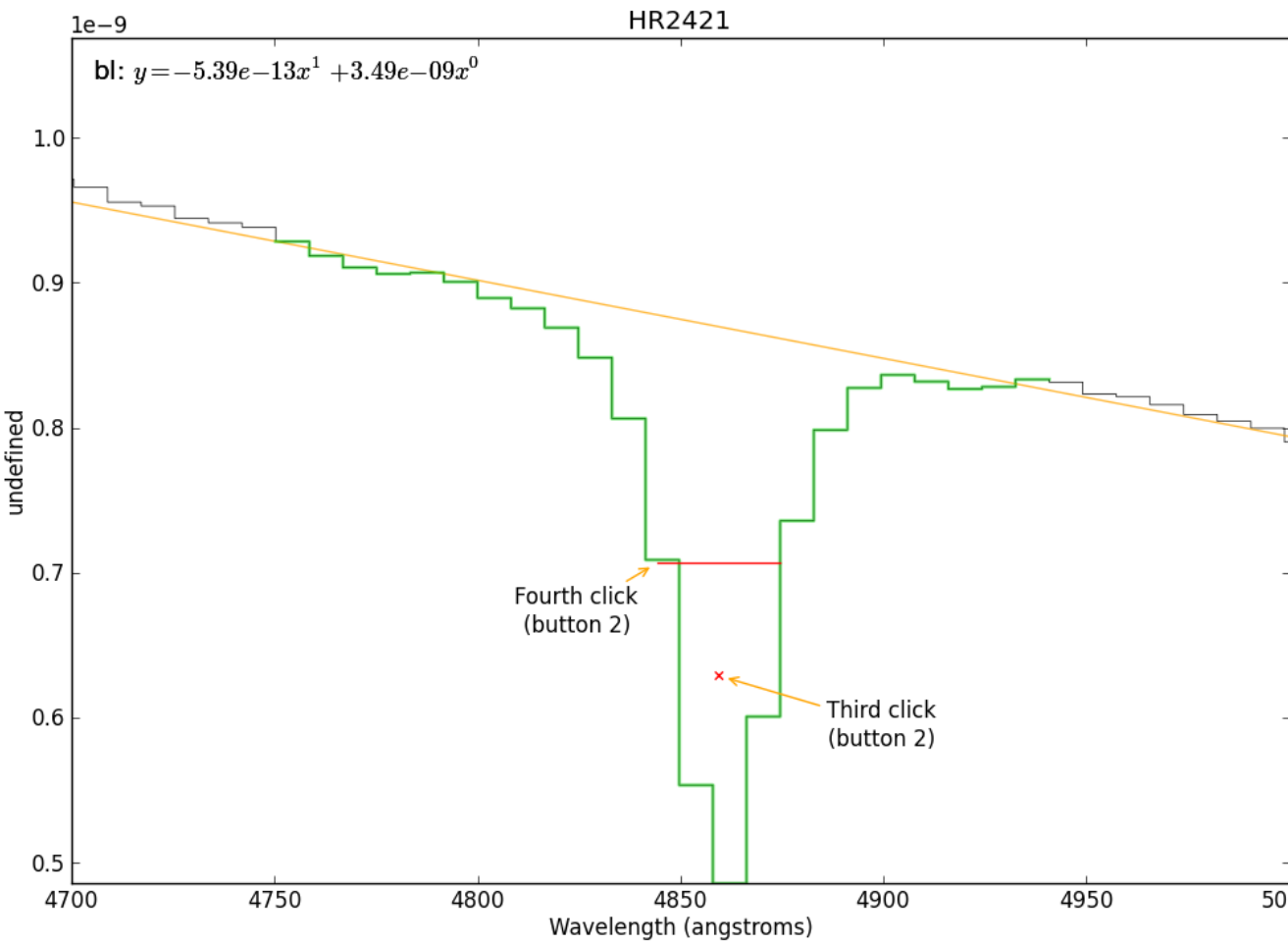


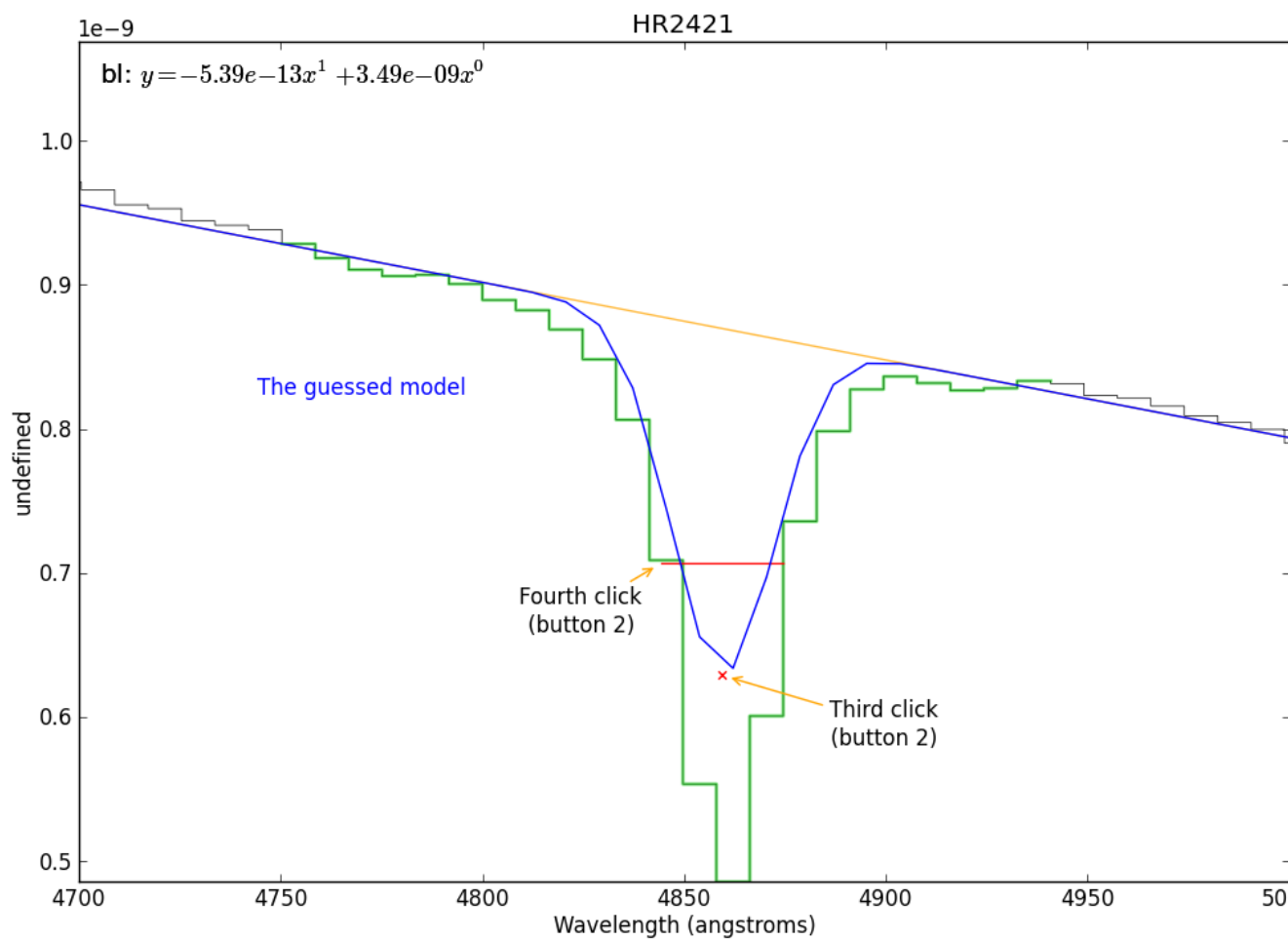




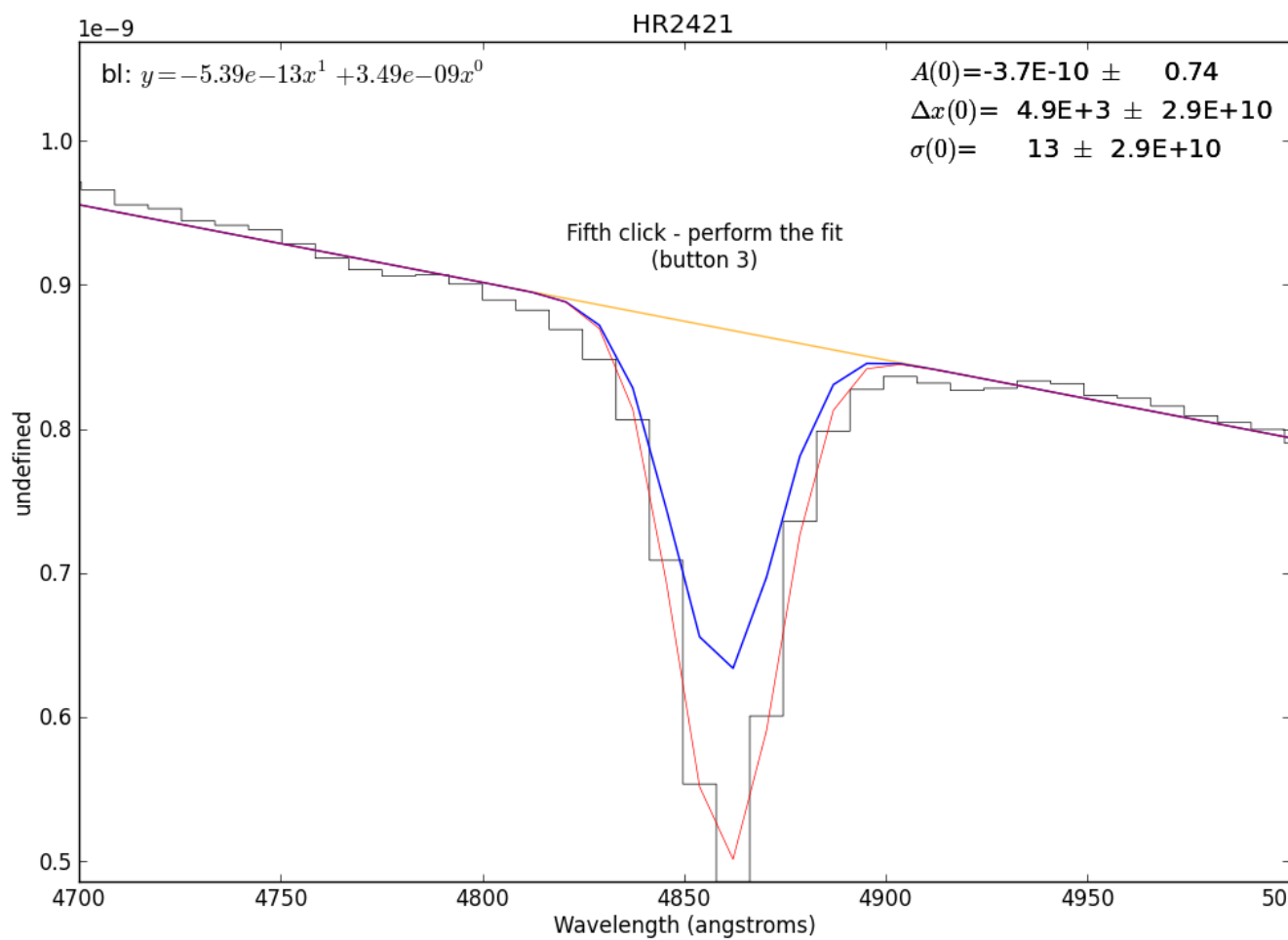












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```

0.11957267912208754, 6678.3853431367716, 4.1892742162283181, 1,
0.10506431180136294, 6589.9310414408683, 72.378997529374672, 1,],
fittype='voigt')

# Now overplot the fitted components with an offset so we can see them
# the add_baseline=True bit means that each component will be displayed
# with the "Continuum" added
# If this was off, the components would be displayed at y=0
# the component_yoffset is the offset to add to the continuum for plotting
# only (a constant)
sp.specfit.plot_components(add_baseline=True, component_yoffset=-0.2)

# Now overplot the residuals on the same graph by specifying which axis to overplot it on
# clear=False is needed to keep the original fitted plot drawn
# yoffset is the offset from y=zero
sp.specfit.plot_residuals(axis=sp.plotter.axis, clear=False, yoffset=0.20, label=False)

# save the figure
sp.plotter.savefig("SN2009ip_UT121002_Halpha_voigt_zoom.png")

```

```

# print the fit results in table form
# This includes getting the equivalent width for each component using sp.specfit.EQW
print(" ".join(["%15s %15s" % (s, s+"err") for s in sp.specfit.parinfo.parnames]),
      " ".join(["%15s" % ("EQW"+str(i)) for i, w in enumerate(sp.specfit.EQW(components=True))]))
print(" ".join(["%15g %15g" % (par.value, par.error) for par in sp.specfit.parinfo]),
      " ".join(["%15g" % w for w in sp.specfit.EQW(components=True)]))

# zoom in further for a detailed view of the profile fit
sp.plotter.axis.set_xlim(6562-150, 6562+150)
sp.plotter.savefig("SN2009ip_UT121002_Halpha_voigt_zoomzoom.png")

```

```

# now we'll re-do the fit with the He I line subtracted off
# first, create a copy of the spectrum
just_halpha = sp.copy()

# Second, subtract off the model fit for the He I component
# (identify it by looking at the fitted central wavelengths)
just_halpha.data -= sp.specfit.modelcomponents[2,:]

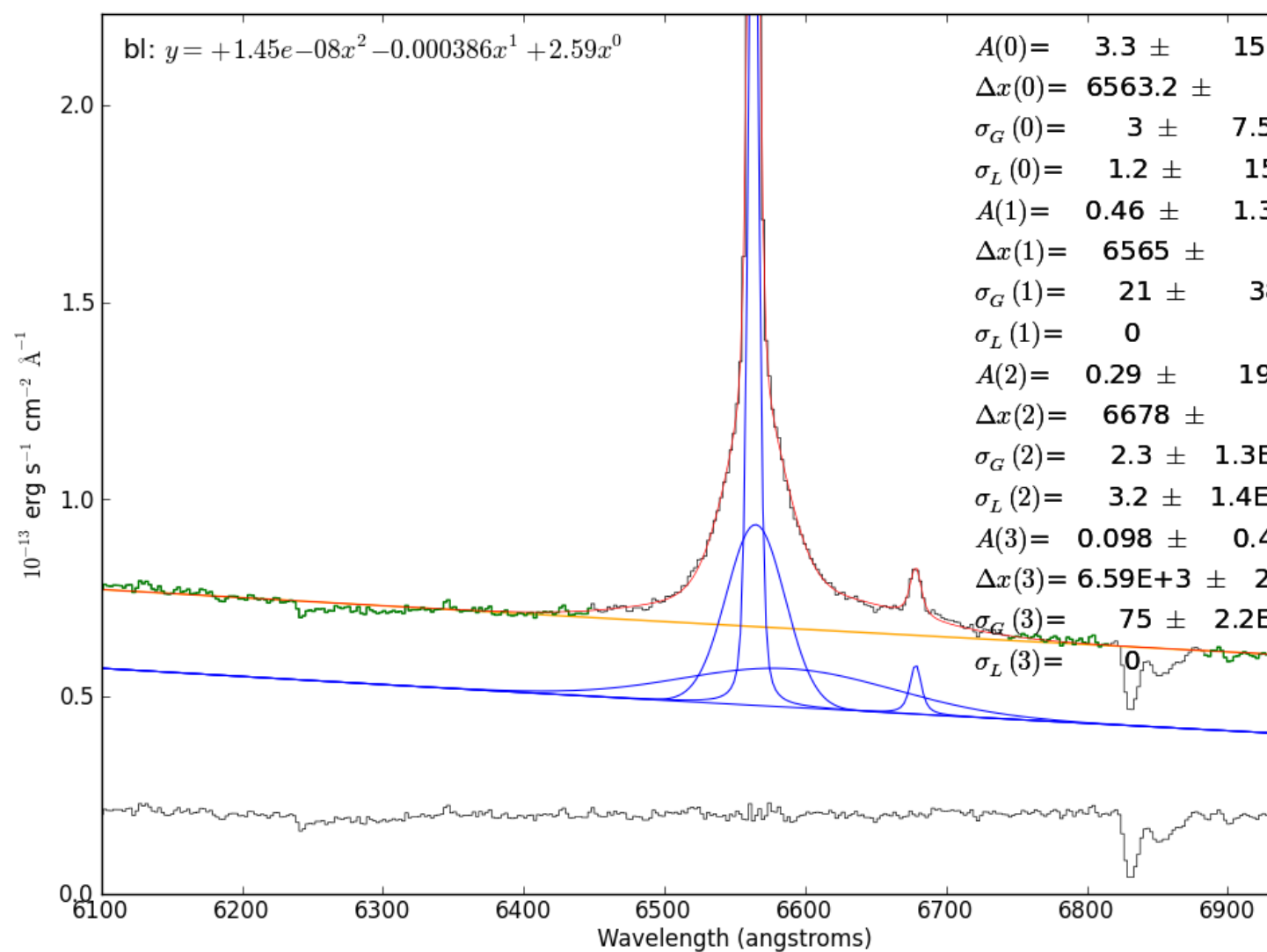
# re-plot
just_halpha.plotter(xmin=6100, xmax=7000, ymax=2.00, ymin=-0.3)

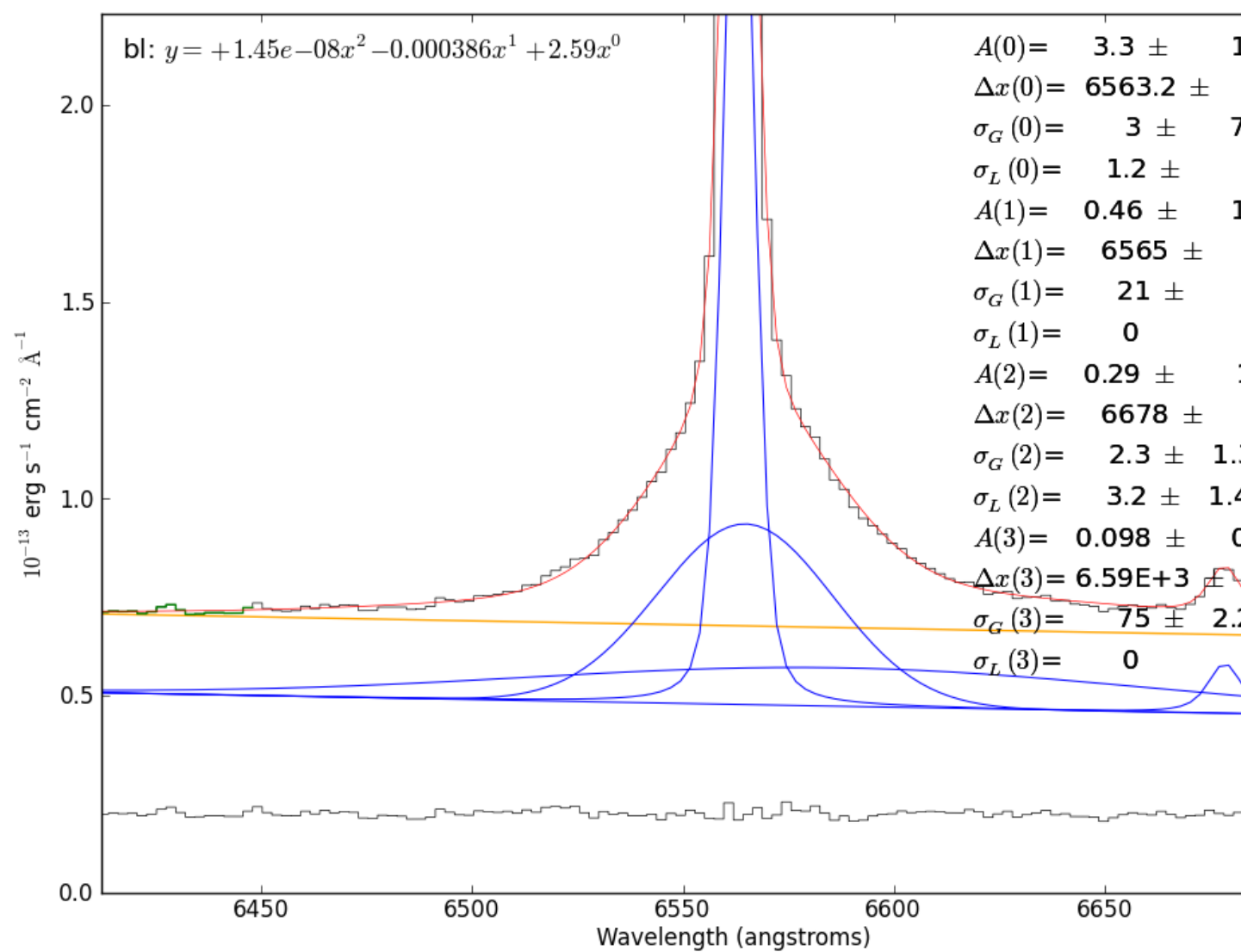
# this time, subtract off the baseline - we're now confident that the continuum
# fit is good enough
just_halpha.baseline(xmin=6100, xmax=7000,
                    exclude=[6450, 6746, 6815, 6884, 7003, 7126, 7506, 7674, 8142, 8231],
                    subtract=True, reset_selection=True, highlight_fitregion=True, order=2)

# Do a 3-component fit now that the Helium line is gone
# I've added some limits here because I know what parameters I expect of my fitted line
just_halpha.specfit(guesses=[2.4007096541802202, 6563.2307968382256, 3.5653446153950314, 1,
                             0.53985149324131965, 6564.3460908526877, 19.443226155616617, 1,
                             0.10506431180136294, 6589.9310414408683, 50.378997529374672, 1,],
                    fittype='voigt',
                    xmin=6100, xmax=7000,
                    limitedmax=[False, False, True, True]*3,

```

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```

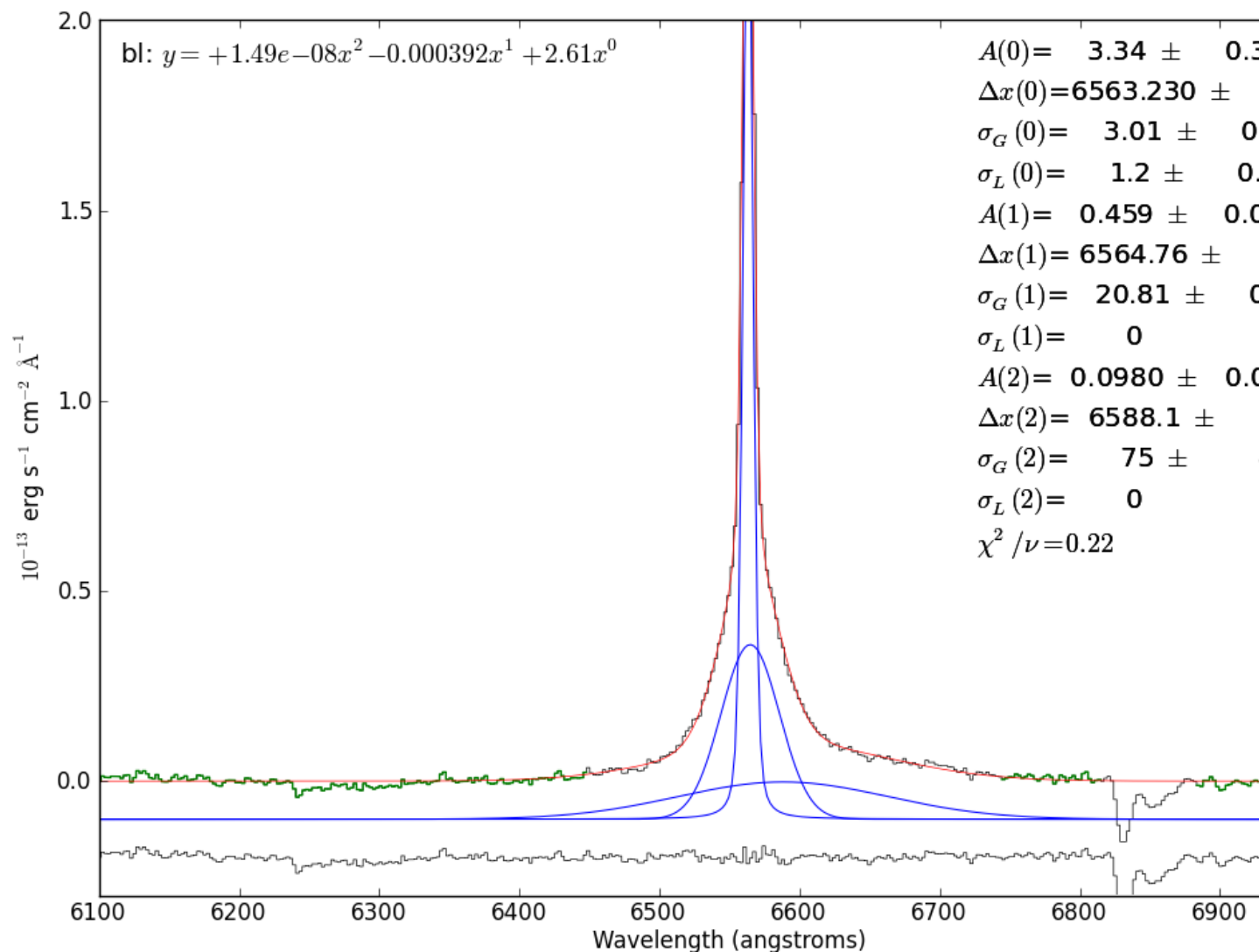
        limitedmin=[True,False,True,True]*3,
        limits=[(0,0),(0,0),(0,100),(0,100)]*3)

# overplot the components and residuals again
just_halpha.specfit.plot_components(add_baseline=False,component_yoffset=-0.1)
just_halpha.specfit.plotresiduals(axis=just_halpha.plotter.axis,
                                  clear=False, yoffset=-0.20, label=False)

# The "optimal chi^2" isn't a real statistical concept, it's something I made up
# However, I think it makes sense (but post an issue if you disagree!):
# It uses the fitted model to find all pixels that are above the noise in the spectrum
# then computes chi^2/n using only those pixels
just_halpha.specfit.annotate(chi2='optimal')

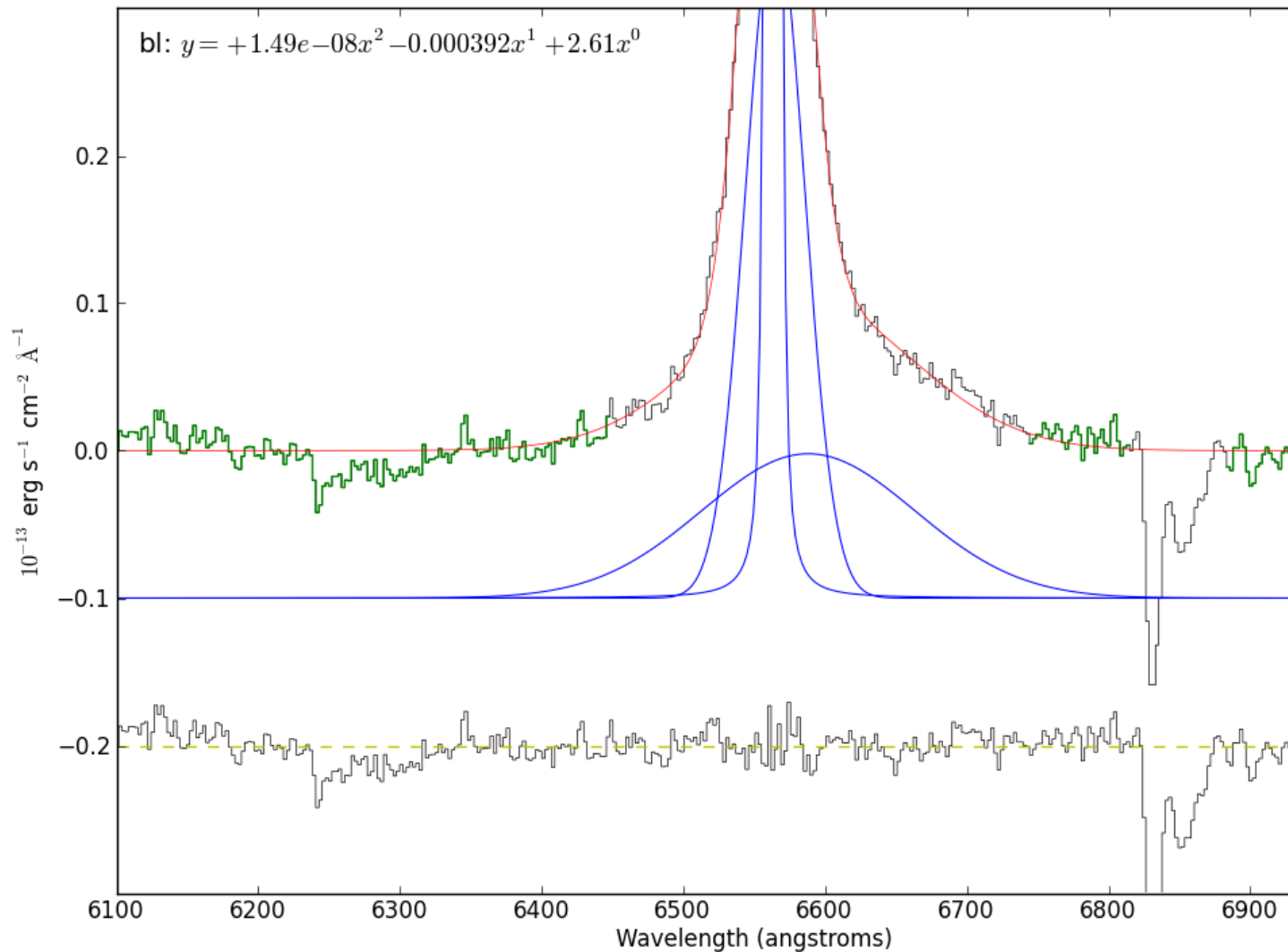
# save the figure
just_halpha.plotter.savefig("SN2009ip_UT121002_Halpha_voigt_threecomp.png")

```



```
# A new zoom-in figure
import pylab

# now hide the legend
just_halpha.specfit.fitleg.set_visible(False)
# overplot a y=0 line through the residuals (for reference)
pylab.plot([6100,7000],[-0.2,-0.2],'y--')
# zoom vertically
pylab.gca().set_ylim(-0.3,0.3)
# redraw & save
pylab.draw()
just_halpha.plotter.savefig("SN2009ip_UT121002_Halpha_voigt_threecomp_zoom.png")
```



```
# Part of the reason for doing the above work is to demonstrate that a
# 3-component fit is better than a 2-component fit
#
# So, now we do the same as above with a 2-component fit

just_halpha.plotter(xmin=6100,xmax=7000,ymax=2.00,ymin=-0.3)
```

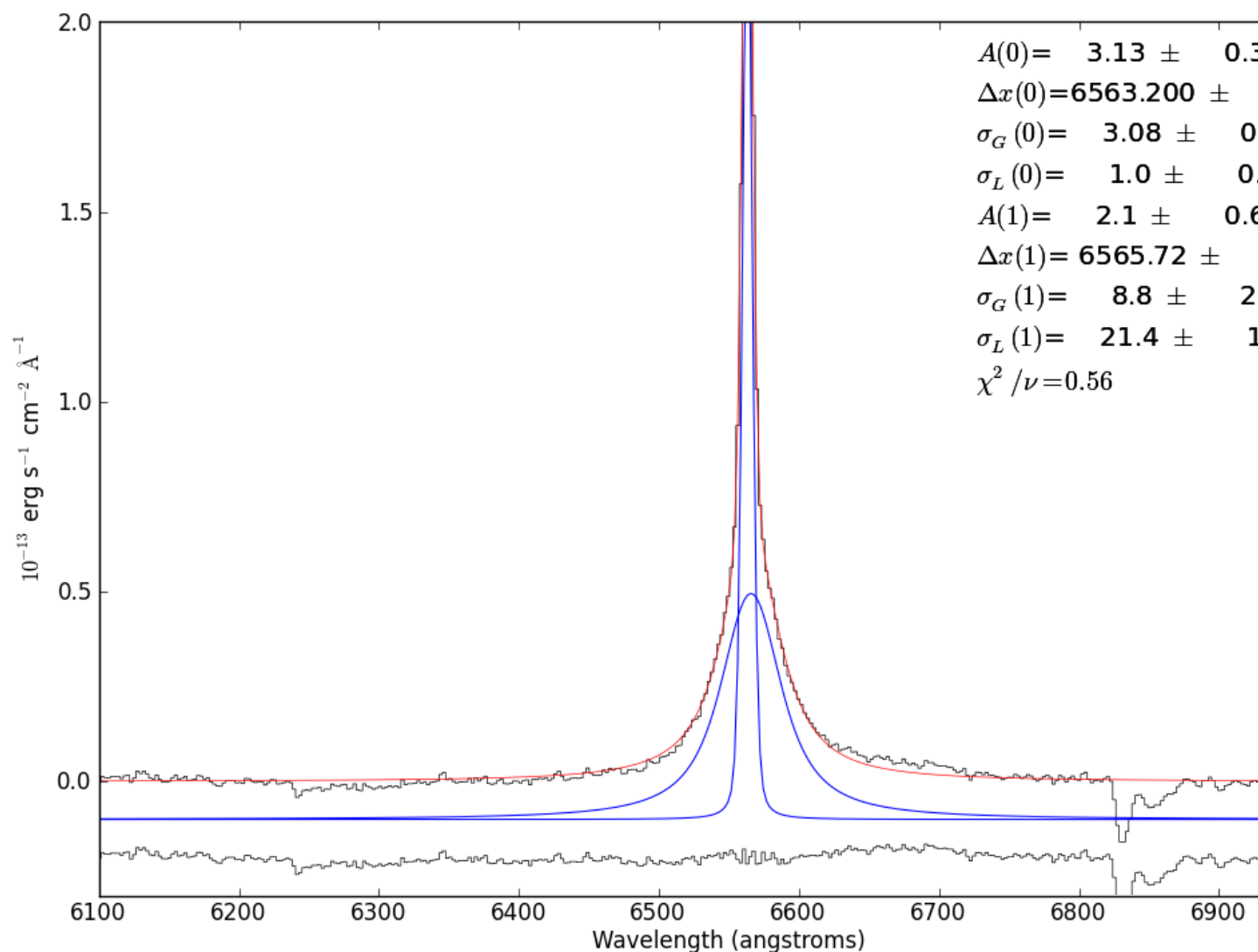
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```

just_halpha.specfit(guesses=[2.4007096541802202, 6563.2307968382256, 3.5653446153950314, 1,
                             0.53985149324131965, 6564.3460908526877, 19.443226155616617, 1],
                    fittype='voigt')
just_halpha.specfit.plot_components(add_baseline=False, component_yoffset=-0.1)
just_halpha.specfit.plotresiduals(axis=just_halpha.plotter.axis,
                                   clear=False, yoffset=-0.20, label=False)
just_halpha.specfit.annotate(chi2='optimal')
just_halpha.plotter.savefig("SN2009ip_UT121002_Halpha_voigt_twocomp.png")

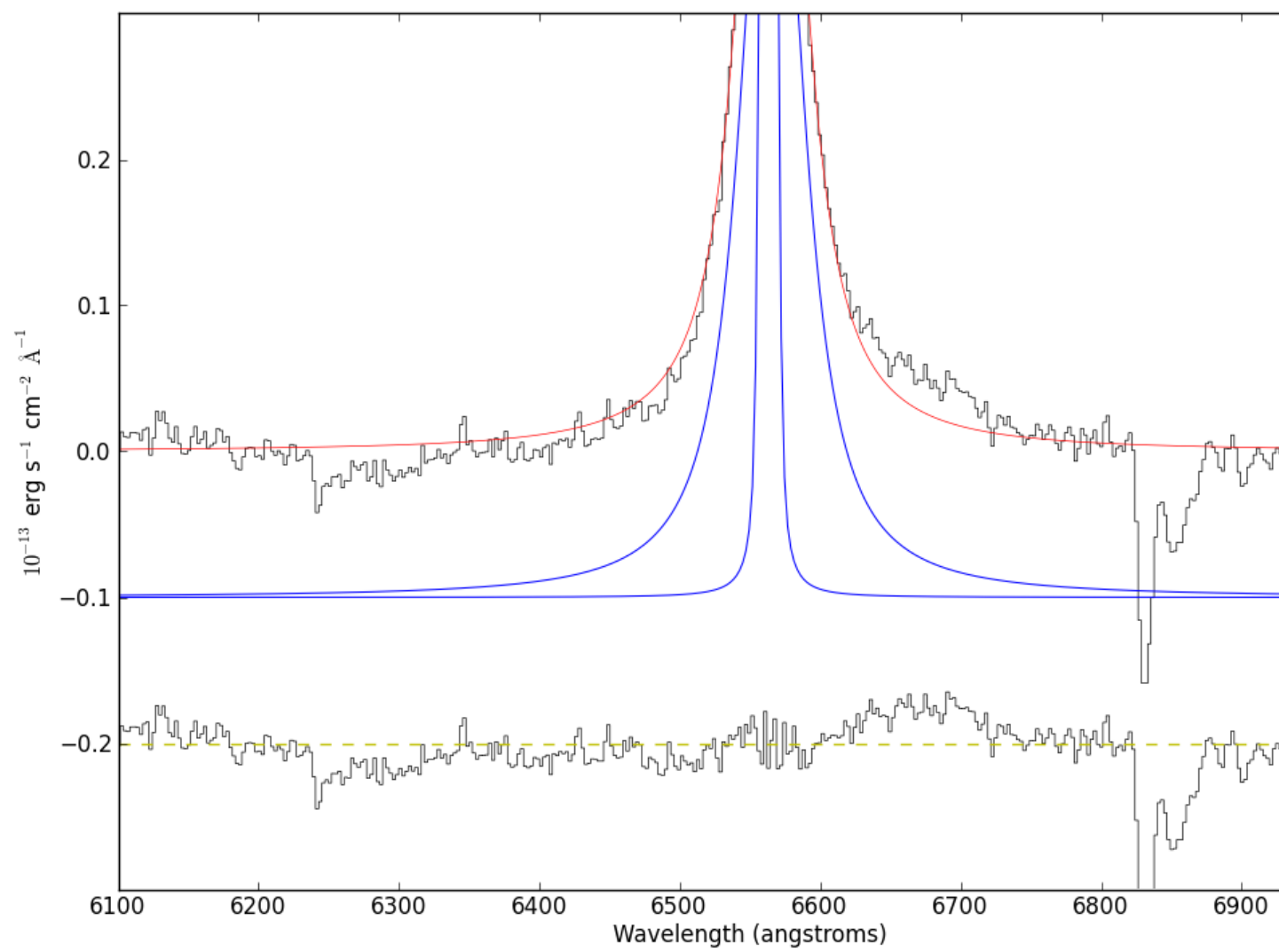
```



```

just_halpha.specfit.fitleg.set_visible(False)
pylab.plot([6100, 7000], [-0.2, -0.2], 'y--')
pylab.gca().set_ylim(-0.3, 0.3)
pylab.draw()
just_halpha.plotter.savefig("SN2009ip_UT121002_Halpha_voigt_twocomp_zoom.png")

```





## 8.19 MUSE cube fitting

An example analysis of a MUSE data cube using both `spectral_cube` and `pyspeckit`

```
from astropy.io import fits
from astropy import units as u
import numpy as np
import spectral_cube
import pyspeckit
from spectral_cube.spectral_axis import vac_to_air

lines = {'OI6300': 6302.046,
         'SIII6313': 6313.8,
         'OI6363': 6365.536,
         'NII6548': 6549.85,
         'HAlpha': 6564.61,
         'HBeta': 4862.69,
         'NII6584': 6585.28,
         'HeI6678': 6679.99556,
         'SII6716': 6718.29,
         'SII6731': 6732.67,
         'pa20': 8394.71,
         'pa19': 8415.63,
         'pa18': 8440.27,
         'pa17': 8469.59,
         'pa16': 8504.83,
         'pa15': 8547.73,
         'pa14': 8600.75,
         'pa13': 8667.40,
         'pa12': 8752.86,
         'pa11': 8865.32,
         'pa10': 9017.8,
         'pa9': 9232.2,
         'HeI7067': 7067.138,
         'HeI7283': 7283.355,
         'ArIII7135': 7137.8,
         'ArIII7751': 7753.2,
         'SIII9071': 9071.1,
         'NeII5756': 5756.24,
         'HeI5877': 5877.3,
         'OIII5008': 5008.24,
         'OII4960': 4960.3,
        }

# use spectral_cube to read the data
cube = spectral_cube.SpectralCube.read('CUBEec_nall.fits', hdu=1)
cont = cube.spectral_slab(6380*u.AA, 6500*u.AA).apply_numpy_function(np.mean, axis=0)

# "slabs" are velocity-cutouts of the cube
# Cube velocity conversion should use vacuum wavelengths
slabs = {line:
         cube.with_spectral_unit(u.km/u.s, velocity_convention='optical',
                                rest_value=w1*u.AA)
         .spectral_slab(-200*u.km/u.s, 250*u.km/u.s)
         for line,w1 in lines.items()}

# Compute 1st moments (intensity-weighted velocity)
```

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```

for line,slab in slabs.items():
    print "kms",line
    mom1 = slab.moment1(axis=0)
    mom1.write('moments/moment1_125_{0}_kms.fits'.format(line), overwrite=True)
mean_moment = np.mean([fits.getdata('moments/moment1_125_{0}_kms.fits'.format(line)) for
                        line in slabs], axis=0)
hdr = fits.getheader('moments/moment1_125_{0}_kms.fits'.format(line))
outfilename = 'moments/moment1_125_mean_kms.fits'
if astropy.version.major >= 2 or (astropy.version.major==1 and astropy.version.minor>=3):
    fits.PrimaryHDU(data=mean_moment, header=hdr).writeto(outfilename, overwrite=True)
else:
    fits.PrimaryHDU(data=mean_moment, header=hdr).writeto(outfilename, clobber=True)

# Create a cube of many different lines all in velocity
# This will allow us to measure a velocity more accurate than is possible
# with one line alone (assuming all lines have the same velocity) because
# MUSE undersamples its line-spread-function a little
newcube_shape = (sum(s.shape[0] for s in slabs.values()),) + slabs.values()[0].shape[1:]
newcube_spaxis = np.concatenate([s.spectral_axis
                                for s in slabs.values()]).value*u.km/u.s
sortvect = newcube_spaxis.argsort()
sortspaxis = newcube_spaxis[sortvect]

newcube = np.empty(newcube_shape)

# normalize each spectrum
ind = 0
for ii,slab in enumerate(slabs.values()):
    data = (slab.filled_data[:] - cont) / (slab.sum(axis=0) - cont*slab.shape[0])
    newcube[ind:ind+data.shape[0], :, :] = data
    ind += data.shape[0]

supercube = newcube[sortvect, :, :]

# Create a pyspeckit cube so we can then fit a gaussian to each spectrum
pxarr = pyspeckit.units.SpectroscopicAxis(sortspaxis.value, units='km/s')
pcube = pyspeckit.Cube(cube=supercube, xarr=pxarr)

# more cores = more faster
pcube.fiteach(fittype='gaussian', guesses=[1/np.sqrt(np.pi), 10, 50.0],
             errmap=np.ones(supercube.shape[1:])/10., multicore=40)

pcube.write_fit('velocity_fits_125.fits', overwrite=True)

```

## 8.20 Fitting using a Template

Pyspeckit allows you to use a spectral template as the model to fit to your spectrum. See `pyspeckit.spectrum.models.template`.

If your model spectrum only requires a shift and a scale, it's easy to use:

```

from pyspeckit.spectrum.models.template import template_fitter

template = pyspeckit.Spectrum('template_spectrum.fits')

```

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```

dataspec = pyspeckit.Spectrum("DataSpectrum.fits")

# Create the fitter from the template spectrum and "Register" it
template_fitter = template_fitter(template,xshift_units='angstroms')
dataspec.Registry.add_fitter('template',template_fitter,2)

# The fitted parameters are amplitude & xshift
# perform the fit:
dataspec.specfit(fittype='template',guesses=[1,0])

# print the results
print dataspec.specfit.parinfo

```

## 8.21 Monte Carlo examples

There are (at least) two packages implementing Monte Carlo sampling available in python: `pymc` and `emcee`. `pyspeckit` includes interfaces to both. With the `pymc` interface, it is possible to define priors that strictly limit the parameter space. So far that is not possible with `emcee`.

The examples below use a custom plotting package from `agpy`. It is a relatively simple but convenient wrapper around `numpy`'s `histogram2d`. `pymc_plotting` takes care of indexing, percentile determination, and coloring.

The example below shows the results of a gaussian fit to noisy data ( $S/N \sim 6$ ). The parameter space is then explored with `pymc` and `emcee` in order to examine the correlation between width and amplitude.

```

import pyspeckit
import numpy as np

# Create our own gaussian centered at 0 with width 1, amplitude 5, and
# gaussian noise with amplitude 1
x = pyspeckit.units.SpectroscopicAxis(np.linspace(-10,10,50), unit='km/s')
e = np.random.randn(50)
d = np.exp(-np.asarray(x)**2/2.)*5 + e

# create the spectrum object
sp = pyspeckit.Spectrum(data=d, xarr=x, error=np.ones(50)*e.std())
# fit it
sp.specfit(fittype='gaussian', guesses=[1,0,1])
# then get the pymc values
MCuninformed = sp.specfit.get_pymc()
MCwithpriors = sp.specfit.get_pymc(use_fitted_values=True)
MCuninformed.sample(101000,burn=1000,tune_interval=250)
MCwithpriors.sample(101000,burn=1000,tune_interval=250)

# MC vs least squares:
print(sp.specfit.parinfo)
# Param #0    AMPLITUDE0 =          4.51708 +/-          0.697514
# Param #1      SHIFT0 =          0.0730243 +/-          0.147537
# Param #2     WIDTH0 =          0.846578 +/-          0.147537   Range:   [0,inf)

print(MCuninformed.stats()['AMPLITUDE0'],MCuninformed.stats()['WIDTH0'])
# {'95% HPD interval': array([ 2.9593463 ,  5.65258618]),
#   'mc error': 0.0069093803546614969,

```

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```

# 'mean': 4.2742994714387068,
# 'n': 100000,
# 'quantiles': {2.5: 2.9772782318342288,
# 25: 3.8023115438555615,
# 50: 4.2534542126311479,
# 75: 4.7307441549353229,
# 97.5: 5.6795448148793293},
# 'standard deviation': 0.68803712503362213},
# {'95% HPD interval': array([ 0.55673242,  1.13494423]),
# 'mc error': 0.0015457954546501554,
# 'mean': 0.83858499779600593,
# 'n': 100000,
# 'quantiles': {2.5: 0.58307734425381375,
# 25: 0.735072721596429,
# 50: 0.824695077252244,
# 75: 0.92485225882530664,
# 97.5: 1.1737067304111048},
# 'standard deviation': 0.14960171537498618}

print(MCwithpriors.stats()['AMPLITUDE0'],MCwithpriors.stats()['WIDTH0'])
# {'95% HPD interval': array([ 3.45622857,  5.28802497]),
# 'mc error': 0.0034676818027776788,
# 'mean': 4.3735547007147595,
# 'n': 100000,
# 'quantiles': {2.5: 3.4620369729291913,
# 25: 4.0562790782065052,
# 50: 4.3706408236777481,
# 75: 4.6842793868186332,
# 97.5: 5.2975444315549947},
# 'standard deviation': 0.46870135068815683},
# {'95% HPD interval': array([ 0.63259418,  1.00028015]),
# 'mc error': 0.00077504289680683364,
# 'mean': 0.81025043433745358,
# 'n': 100000,
# 'quantiles': {2.5: 0.63457050661326331,
# 25: 0.7465422649464849,
# 50: 0.80661741451336577,
# 75: 0.87067288601310233,
# 97.5: 1.0040591994661381},
# 'standard deviation': 0.093979950317277294}

# optional
from mpl_plot_templates import pymc_plotting
import pylab
pymc_plotting.hist2d(MCuninformed, 'AMPLITUDE0', 'WIDTH0', clear=True, bins=[25,25])
pymc_plotting.hist2d(MCwithpriors, 'AMPLITUDE0', 'WIDTH0', contourcmd=pylab.contour, colors=[(0,1,0,1),(0,0.5,1),(0,0.75,0.75,1),(0,1,1,1),(0,0,1,1)], clear=False, bins=[25,25])
pylab.plot([5],[1], 'k+', markersize=25, zorder=1000)
pylab.savefig("pymc_example_Gaussian_amplitude_vs_width.pdf")

# Now do the same with emcee
emcee_ensemble = sp.specfit.get_emcee()
p0 = emcee_ensemble.p0 * (np.random.randn(*emcee_ensemble.p0.shape) / 10. + 1.0)
pos, logprob, state = emcee_ensemble.run_mcmc(p0, 100000)

```

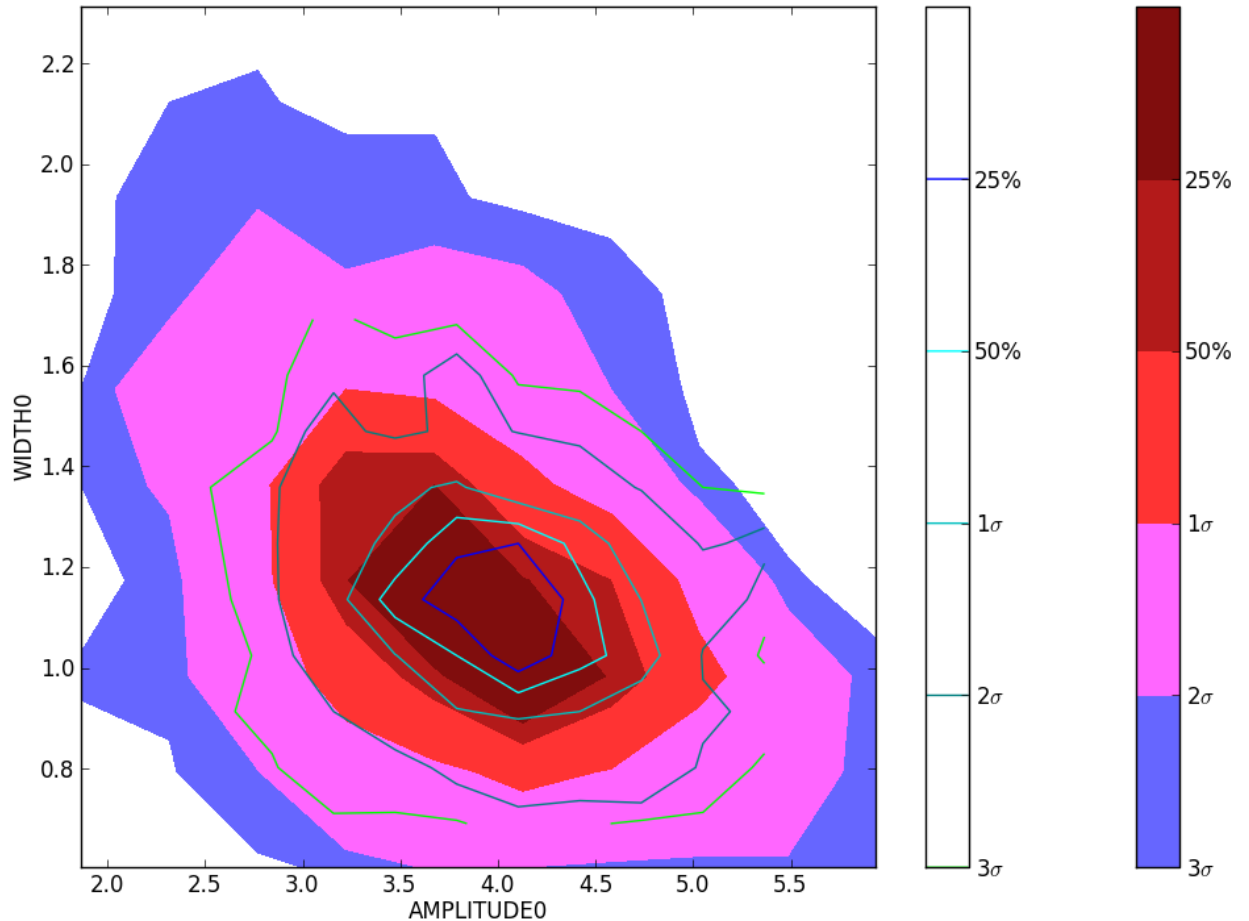
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```

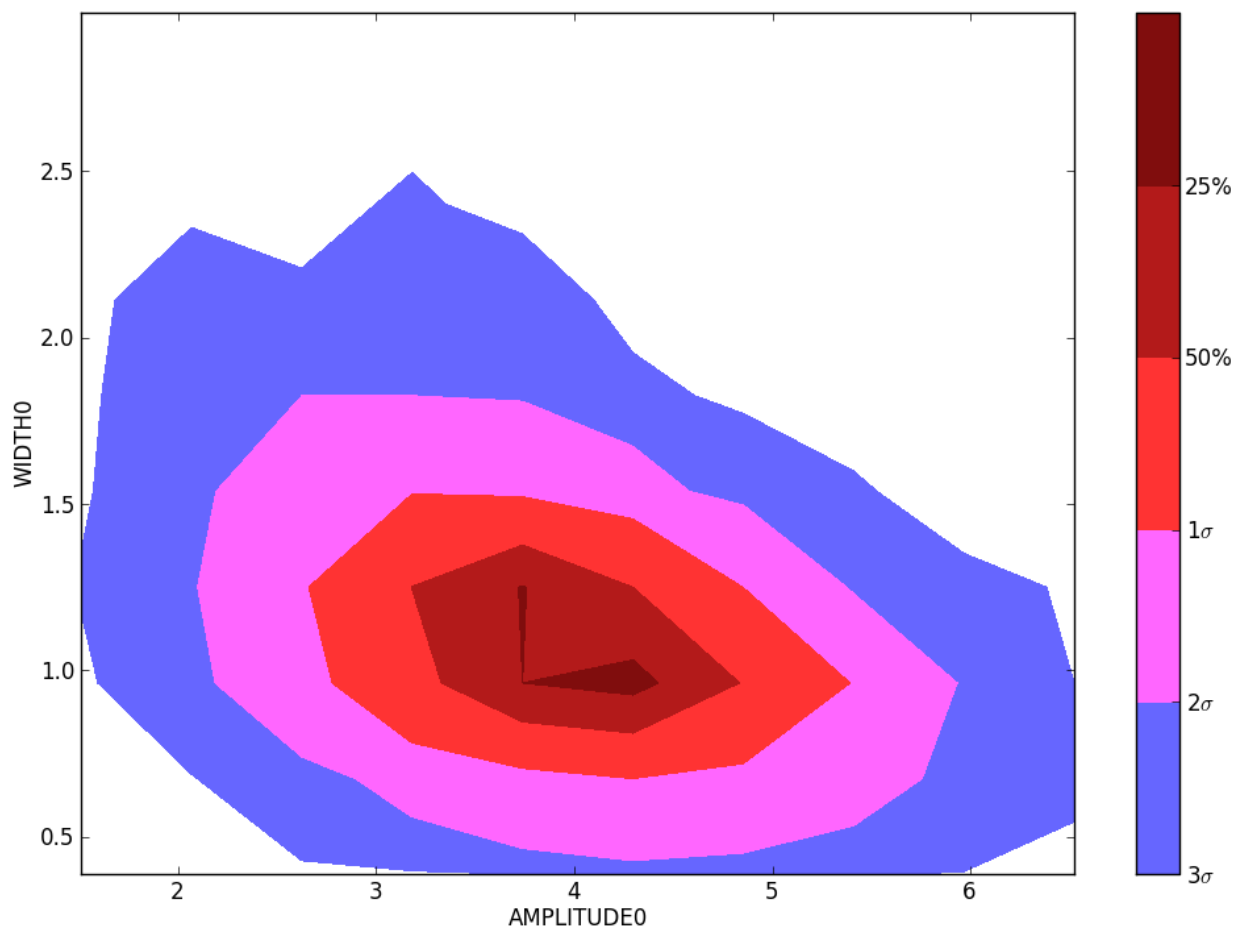
plotdict = {'AMPLITUDE0':emcee_ensemble.chain[:,0].ravel(),
            'WIDTH0':emcee_ensemble.chain[:,2].ravel()}
pymc_plotting.hist2d(plotdict, 'AMPLITUDE0', 'WIDTH0', fignum=2, bins=[25,25], clear=True)
pylab.plot([5],[1], 'k+', markersize=25)
pylab.savefig("emcee_example_Gaussian_amplitude_vs_width.pdf")

```



The Amplitude-Width parameter space sampled by pymc with (lines) and without (solid) priors. There is moderate anticorrelation between the line width and the peak amplitude. The + symbol indicates the input parameters; the model does a somewhat poor job of recovering the true values (in case you're curious, there is no intrinsic bias - if you repeat the above fitting procedure a few hundred times, the mean fitted amplitude is 5.0).

The parameter space sampled with emcee and binned onto a 25x25 grid. Note that emcee has 6x as many points (and takes about 6x as long to run) because there are 6 “walkers” for the 3 parameters being fit.



## 8.22 Ammonia Monte Carlo examples

This example shows the same process as in [example\\_pymc](#), but for the ammonia model. Here we emphasize the degeneracy between the excitation temperature and the total column density.

```
import numpy as np
from astropy import units as u
import itertools
from operator import itemgetter
import pyspeckit
import scipy.stats

from pyspeckit.spectrum.models import ammonia, ammonia_constants

import pylab as pl
pl.close('all')
pl.figure(1).clf()

oneonefreq = ammonia_constants.freq_dict['oneone']
twotwofreq = ammonia_constants.freq_dict['twotwo']
# create an axis that covers the 1-1 and 2-2 inversion lines
xaxis = pyspeckit.units.SpectroscopicAxis(np.linspace(oneonefreq*(1-50/3e5),
                                                    twotwofreq*(1+50/3e5),
                                                    1000.),
                                           unit=u.Hz)

sigma = 2.
center = 0.
trot = 15.
ntot = 14.7
# Adopting an NLTE model: T_ex < T_rot (this case is better for the default fitter)
# pyradex.Radex(species='p-nh3', column=5e14, collider_densities={'h2':5000}, temperature=15())[8:10]
tex = {'oneone':8.5, 'twotwo':5.5}
synth_data = ammonia.ammonia(xaxis, trot=trot, tex=tex, width=sigma,
                             xoff_v=center, ntot=ntot)

# Add noise
stddev = 0.1
noise = np.random.randn(xaxis.size)*stddev
error = stddev*np.ones_like(synth_data)
data = u.Quantity(noise+synth_data, u.K)

# create the spectrum object
sp = pyspeckit.Spectrum(data=data,
                        xarr=xaxis,
                        error=np.ones_like(synth_data)*stddev)

# fit it
# Setting limits is important for running the MCMC chains below (they set the
# priors)
sp.specfit(fittype='ammonia',
           # trot, tex, ntot, width, center, fortho
           guesses=[35,10,15,5,5,0],
           fixed=[False,False,False,False,False,True],
           minpars=[3,3,10,0,-10,0],
           maxpars=[80,80,20,10,10,1],
           limitedmin=[True]*6,
           limitedmax=[True]*6,
           )
```

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```

# then get the pymc values
MCUniformpriors = sp.specfit.get_pymc()
MCUniformpriors.sample(10100, burn=100, tune_interval=250)

# MC vs least squares:
print(sp.specfit.parinfo)

print(MCUniformpriors.stats()['tex0'],
      MCUniformpriors.stats()['ntot0'])

# optional plotting
from mpl_plot_templates import pymc_plotting
import pylab
pylab.figure(1).clf()
pymc_plotting.hist2d(MCUniformpriors, 'tex0', 'ntot0',
                    bins=[25,25])
pylab.plot([tex['oneone']], [ntot], 'k+', markersize=25)
pylab.axis([6, 10.5, 14.6, 14.9])
pylab.savefig("tex_vs_ntot_pymc_example.pdf")

# Now do the same with emcee
emcee_ensemble = sp.specfit.get_emcee()
p0 = emcee_ensemble.p0 * (np.random.randn(*emcee_ensemble.p0.shape) / 50. + 1.0)
pos, logprob, state = emcee_ensemble.run_mcmc(p0, 10000)

plotdict = {'tex0': emcee_ensemble.chain[:, 1000:, 1].ravel(),
            'ntot0': emcee_ensemble.chain[:, 1000:, 2].ravel()}
# one of the samplers went off the hook and got locked at high ntot
OK = (plotdict['ntot0'] < 20)
plotdict['tex0'] = plotdict['tex0'][OK]
plotdict['ntot0'] = plotdict['ntot0'][OK]

pylab.figure(2).clf()
pymc_plotting.hist2d(plotdict, 'tex0', 'ntot0', fignum=2, bins=[25,25],
                    clear=True)
pylab.plot([tex['oneone']], [ntot], 'k+', markersize=25)
pylab.axis([6, 10.5, 14.6, 14.9])
pylab.savefig("tex_vs_ntot_emcee_example.pdf")

```

## 8.23 Guide for GILDAS-CLASS users

### 8.23.1 Reading Files

PySpecKit can read many file types including CLASS .cls files.

For example, a typical single-dish observing file will consist of a large number of individual spectra. These may be on-the-fly spectra or multiple integrations on a single source; either way the pointing and spectral information for each individual data point should be incorporated in the data file.

The spectra are recorded from the data file into an `pyspeckit.classes.ObsBlock` object. An `ObsBlock` (Observation Block) is simply a container for many spectra; in most regards it behaves the same way as a `pyspeckit.Spectrum` object, but it has a few extra attributes built-in (e.g., spectral averaging).



A file can be loaded as a named object. The data is filtered as it is read in. The following line will ensure that the spectra in the n2hp ObsBlock contain only data from the F1M spectrometer with lines labeled 'N2HP(3-2)' or 'N2H+(3-2)':

```
from pyspeckit.spectrum.readers.read_class import class_to_obsblocks
n2hp = class_to_obsblocks(filename,
    telescope=['SMT-F1M-HU', 'SMT-F1M-VU'],
    line=['N2HP(3-2)', 'N2H+(3-2)'])
```

### 8.23.2 Working with the data

You can treat an ObsBlock like any other `pyspeckit.Spectrum` object, but there are a few unique features.

The 'smooth' function will smooth each individual spectrum in the ObsBlock, which can be useful if you want to smooth before averaging.

The 'average' function averages spectra. Weights for the averaging can be specified. The error is also computed either by taking the RMS of the averaged spectra or by averaging the error spectra.

You can plot each spectrum in an individual window with the `ploteach` function, or all overlaid simultaneously with the 'plotter' function. If you want to loop through each spectrum, waiting for user input after displaying, you can do something like:

```
ax = pylab.gca()
for sp in n2hp:
    sp.plotter(axis=ax)
    input("Waiting for input...")
```

You can also fit a line profile to *each* spectrum in the observation block using the 'fiteach' command.

### 8.23.3 Selecting Spectra

There are 3 keywords that can be used to select spectra when reading in a file. The line and telescope keywords are required in order to make an observation block, otherwise the spectral axes will not be common to all spectra.:

```
n2hp = class_to_obsblocks(filename,
    telescope=['SMT-F1M-HU', 'SMT-F1M-VU'],
    line=['N2HP(3-2)', 'N2H+(3-2)'])
```

If you want to read in all of the data and don't care about the line or telescope, you can instead use:

```
all_data = class_to_spectra(filename)
```

You can select data after they are read in by matching header keywords:

```
g10 = pyspeckit.ObsBlock([sp for sp in all_data if sp.specname == 'g10'])
```

### 8.23.4 Fitting Data

In CLASS, you would specify the data range with individual commands on the command line, e.g.:

```
[this isn't quite right]
xrange 5 25
```

In pyspeckit, you can specify the range in multiple ways, but the default is to use the plotted window. For example:

```
sp.plotter(xmin=5, xmax=25)
sp.baseline()
sp.specfit()
```

will perform a baseline fit and spectrum fit over the range 5-25 km/s (the units of `xmin`, `xmax` are the plotted units). More intricate specifications are possible:

```
sp.plotter()
# Fit a baseline over the region 5-25 km/s, excluding 7-10 km/s and 15-18 km/s
sp.baseline.selectregion(xmin=5, xmax=25, exclude=[7, 10, 15, 18])
sp.baseline()
sp.specfit()
```

## 8.24 Guide for IRAF users

PySpecKit is similar in intent and implementation to IRAF's *splot* routine. IRAF users will probably want to do most of their data reduction (i.e., turning an image/cube into a 1D wavelength-calibrated spectrum) in IRAF, but will be comfortable fitting lines and making publication-quality plots using PySpecKit.

### 8.24.1 Loading a Spectrum

If you have an IRAF spectrum, it is straightforward to load into PySpecKit:

```
sp = pyspeckit.Spectrum('iraf_spectrum.ms.fits')
sp.plotter()
```

### 8.24.2 Fitting Line Profiles

---

**Note:** See *A guide to interactive fitting* for a comprehensive graphical demonstration of these instructions.

---

In IRAF, a line profile is fitted using *k* to start the fitter, then *k*, *l*, or *v* to perform the fit.

In PySpecKit, the continuum (*baseline*) and line profile are determined separately.

Instead of using a key twice to specify the continuum level, a continuum must be fitted from the data. This is done by pressing *b* to turn on the baseline fitter. Click or press *l* to select baseline regions - they will be highlighted in green. Press *3* to fit the baseline and display it as an orange line.

In PySpecKit, the interactive fitter is started by pressing *f* in the plot window. After pressing *f*, instructions will be provided in the terminal window telling you which line profiles are implemented. Select one of these, or use a gaussian by default.

Select the line fitting region by pressing *l* on either side of the line. Select the peak and full-width-half-maximum of the line by pressing *2* at each of these locations in turn. You may repeat this cycle indefinitely to fit multiple profiles (comparable to IRAF's *deblend* capability). Then, press *3* to perform the fit.

The fitted parameters can be accessed (as variables, or printed) through the `Spectrum.specfit.parinfo` parameter. They will also be displayed in the plot legend.

## 8.25 PySpecKit Projects

A few projects appropriate for a Google Summer of Code or similar are outlined below.

### 8.25.1 Refactor and Expand the pyspeckit modeling tools

Since the development of pyspeckit, there has been substantial progress on a more general class of [modeling tools](#) from [astropy](#). Pyspeckit already has a wide variety of data fitting and modeling tools that can readily be modified to use the astropy modeling formalism.

Details of this project need to be worked out, but will include:

- refactoring `pyspeckit.models` to use `astropy.models`
- building a graphical interface to `astropy.models`

### 8.25.2 Refactor and Expand the Unit Test suite

Pyspeckit is a complicated code suite, which has led to many bugs, particularly in the UI. An improved unit test suite would help prevent or remove these bugs. Such a project would start by breaking down the existing tests, which are really end-to-end tests, into their component units.

The refactor would be to use astropy's wrappers around pytest to make the testing smoother and easier to extend. The current model has tests in a different repository because the data got too big, but we can and should have the *data* in a different repository, but the tests all in one place.

### 8.25.3 Incorporate `astropy.units` into `pyspeckit.units`

*This project was done by an ESO-hosted summer student, Dinos Kousidis.*

This project is at the core of both `pyspeckit` and `specutils`.

The most important base functionality of a spectroscopic toolkit is to be able to convert between different spectroscopic systems, e.g. wavelength<->frequency<->velocity. This can be achieved using [astropy's unit equivalencies](#).

The X-axis unit changes will be straightforward project that should require about 2 weeks to complete. The more complicated and interesting project is creating Y-axis units (i.e., flux units) that appropriately adjust with changes to the X-axis. These would make use of other [astropy](#) unit equivalencies, e.g. the [spectral density](#) equivalency.

The end goal will be to have a `Spectrum` object that will live in `specutils` and be inherited by `pyspeckit`, which will provide the interface to modeling and graphical tools.

Additionally, here are some real-world examples. They are not guaranteed to work, but they show the use of pyspeckit in pipelines and paper-producing code.

- Fit each spectrum in a VLA NH3 6-6 cube (Goddi, Ginsburg, Zhang 2016)
- Fit each spectrum in an Arecibo H2CO 1-1 cube (Ginsburg et al, 2015)
- Crop an ALMA CH3CN cube, then fit each spectrum
- Fit each spectrum in an APEX H2CO 3-2 cube with 1 and 2 components (Ginsburg et al, 2016)
- Compute moments, then fit each spectrum in a MUSE cube (McCleod et al, 2015)
- Fit H2 and BrG in a TripleSpec NIR cube (Youngblood et al, 2016)
- Fit NH3 1-1 and 2-2 spectra for the GBT Ammonia Survey (Pineda, Friesen et al)



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Frequently Asked Questions

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### 9.1 I see “UnitConversionError: ‘km / s’ (speed) and ‘GHz’ (frequency) are not convertible” errors when using the ammonia fitter

For versions of pyspeckit 0.16 (May 2015) and later, pyspeckit uses astropy’s units for the spectroscopic axis. It therefore requires an equivalency to be defined.

To create a SpectroscopicAxis with the appropriate equivalency defined, the axis must have a reference frequency (refX) and a velocity\_convention.:

```
>>> from astropy import units as u
>>> from pyspeckit.spectrum.units import SpectroscopicAxis
>>> import numpy as np
>>> xarr = SpectroscopicAxis(np.linspace(22,24)*u.GHz,
                             refX=23*u.GHz,
                             velocity_convention='radio')
```

If you have loaded a spectrum from file and it doesn’t contain the appropriate metadata (usually a CTYPE in the header), you can set the refX and velocity\_convention manually. The options for velocity\_convention are radio, optical, and relativistic.

For details on the meaning of the various velocity conventions, see [Frank Ghigo’s site](#) or [FITS Paper III](#), especially [table 4](#). For details on the accepted FITS CTYPE keywords, see [FITS Paper III](#). In particular, their [table 1](#) specifies all valid spectral coordinate type codes.



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