

fcc_analyzer: a tool to visualize \mathcal{FC} classes output

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1 Description

`fcc_analyzer` is a python/matplotlib based tool that reads the output from \mathcal{FC} classes (for a TI calculation), namely `fort.21` (assignments) and `fort.18` (spectrum), providing a graphical interface to get the assignments of the each individual transition.

2 Installation

No installation is required, but a proper version of the python interpreter along with numpy and matplotlib modules is needed. The program was developed using the following version of each element:

- python-2.7.5¹
- numpy-1.9.1
- matplotlib-1.4.2

In most distributions, python-2.7 is already included (and is the default), but the modules numpy and matplotlib should be installed. Both modules are already available from Ubuntu or Fedora repositories (among many others), through either:

Listing 1: matplotlib from Ubuntu	Listing 2: matplotlib from Fedora
<code>apt-get install python-matplotlib</code>	<code>yum install python-matplotlib</code>

However, these packaged versions might not be recent enough, and the script may behave wrongly². Therefore, it is advisable to install them from the python setuptools (pip). Below, the installation steps followed in *fresh*³ Ubuntu 14.04 and Fedora 21 distributions are described.

¹This program will **not** work with python-3.

²Attempts with matplotlib-1.3.1 work, but with some capabilities disabled.

³Default installation plus the compilers (gcc, gfortran and g++).

Listing 3: Installing matplotlib in Ubuntu 14.04.

```
#Install python-pip package
apt-get install python-pip
#Install python-dev package
apt-get install python-dev
#Install numpy
pip install numpy
#freetype and png required
apt-get install libfreetype6-dev
#Install matplotlib
pip install matplotlib
```

Listing 4: Installing matplotlib in Fedora 21.

```
#Install python-pip package
yum install python-pip
#Install python-devel package
yum install python-devel
#Install numpy
pip install numpy
#freetype and png required
yum install freetype-devel
#Install matplotlib
pip install numpy
```

After the above, you should have matplotlib-1.4.2 (or above). If not, please, check the documentation of matplotlib, numpy and python in their respective websites. You can use `pip freeze` to see the version of all python modules installed.

3 Using `fcc_analyzer`

After running a TI calculation with *FCclasses*, and on the same folder, type (providing `fcc_analyzer.py` is in your PATH):

```
fcc_analyzer.py
```

This will open a matplotlib plot with all the transition divided by *classes* (read from fort.21) and the final convoluted spectrum (read from fort.18). The following operations are possible:

3.1 Identifying transitions

- **Right-mouse click over a transition:** show assignment of the highlighted transition. The rest of the info for this transition on fort.21 is shown on console.
- **Press '+' or '-' :** browse over the transitions, highlighting the following ('+') or previous ('-') one.
- **Left-mouse click over the legend items (classes):** hide the class on the plot.





3.2 Managing labels

- **Left-mouse click over a transition:** place a label over the transition showing the final modes.
- **Right-mouse click over a label (and hold):** move the label. The pointer line will follow the label.
- **Left-mouse click over a label:** erase the label

3.3 Cleaning

- **Right-mouse click over the plot title:** erase all labels and transition info.
- **Left-mouse click over a plot title:** erase transition info only.

3.4 Using matplotlib functionalities⁴

- **Press 'o' or zoom button,** : zoom into (left mouse click) or out (right mouse click) a rectangle.
- **Press 'p' or move button,** : move the spectrum (left mouse click) or zoom (right mouse click).
- **Press save button,** : export image.
- **Press edit button,** : customize, among others, the plot title.

(Note: mouse-click interactions with the plot are not active in zoom or move modes).

3.5 Export plot to xmgrace

- **Central-mouse click over the plot title:** this will create a xmgrace file called `fcc_analyzer.agr`, containing the convoluted and stick spectra and the labels selected in the plot. The axis ranges are kept.

4 Error messages

- **ERROR: Check 0-0 transition**

The program could not read the intensity for the 0-0 transition on fort.21. In old *FCclasses* versions, there was a bug on the format for this value on fort.21, and it is not printed if it is over 10. You have to insert it manually below SPECTRUM on the 0-0 TRANSITION section of the file. The actual value can be taken from fort.8.

⁴The availability of these options (and the aspect of the buttons) depends on the backend you are using for matplotlib. The ones shown here correspond to *Qt4Agg* backend, which requires PyQt4 module (in Ubuntu and Fedora, it can be installed from the `python-qt4-dev` or `PyQt4-devel` packages.)