Spectrum Simulation Program by Python

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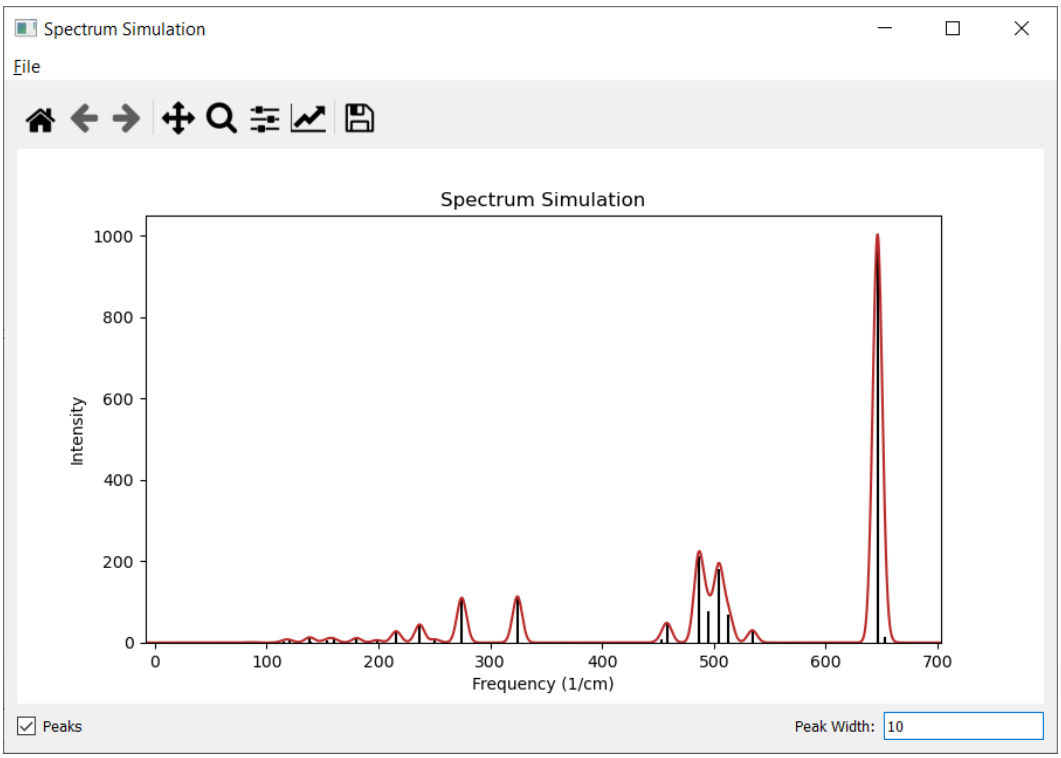
Introduction

This program is a project work for the python programming basic course 2 (CS-A1121, Aalto University) spring 2020.

The spectrum simulation program reads molecule's ideal vibration spectrum (frequency X, intensity Y) from a text file such as:

```
# SrU2F12 Raman spectrum
# X = Freq (cm^-1); Y = Polycrystalline Raman intensity (arb. units)
41.75       0.1
84.27       0.95
88.65       0.0
115.74      3.67
```

and draws the original peaks (black) and the spectrum simulating an experimental spectrum (red):



The user loads a text file through the GUI and can adjust the figure settings and the peak width and visibility. It is also possible to save the figure as a png file.

The peaks of the simulated spectrum are widened using the probability density function of the normal distribution

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} exp\ \frac{(x-x_0)^2}{2\sigma^2}$$

where x0 is the frequency X from the input file and the standard deviation is calculated from the full width at half maximum (FWHM) (https://en.wikipedia.org/wiki/Full_width_at_half_maximum) value (given by the user in the Peak width text field)

$$\sigma = \frac{FWHM}{2\sqrt{2\ln 2}}$$

Single ideal peak (X, Y) is widened by

$$y = Yf(x)$$

However, if the user now changes the peak width (FWHM), f(x) changes and the simulated peak height y is not equal to given peak height Y anymore. In order to fix the value of f(x) to 1, when x=X=x0, it should be scaled. For that the real FWHM, FWHM0, is calculated from the equation

$$f(x) = \frac{2\sqrt{2\ln 2}}{FWHM\sqrt{2\pi}} = 1$$

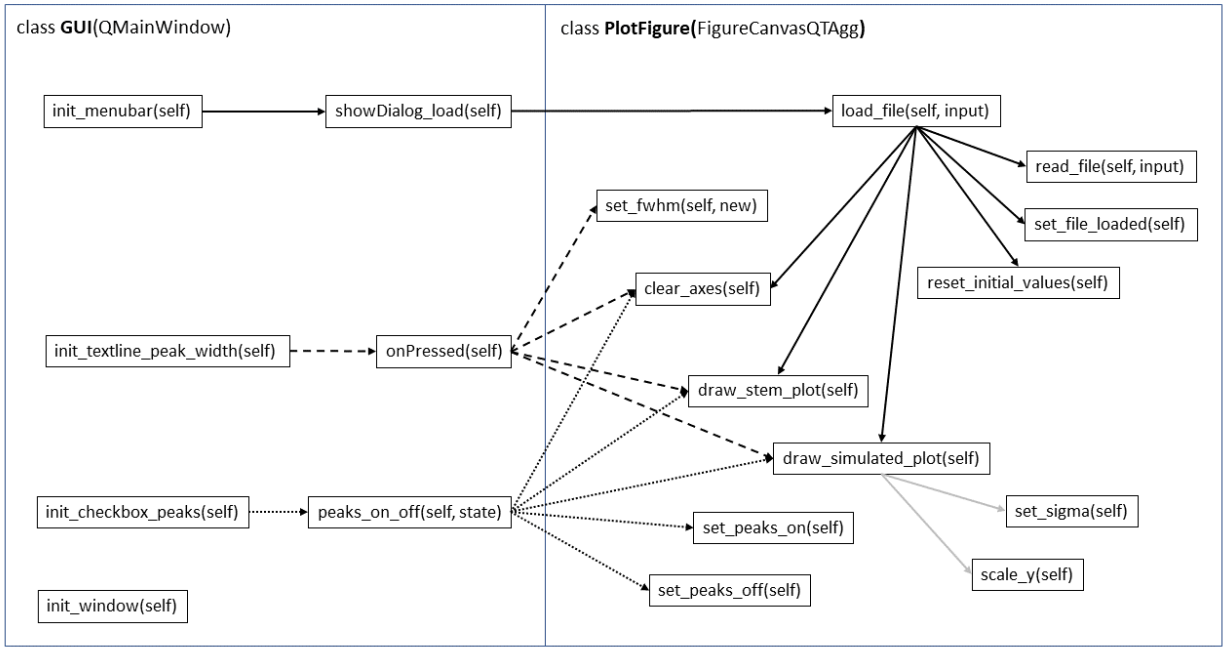
and we get FWHM0≈0,94. If the user changes peak width, f(x) should be scaled by FWHM/FWHM0.

The equation for the simulated spectrum is the sum of all the simulated peaks ysim

$$y_{sim} = \sum y$$

Numpy is used to create the array for plotting the figure, Matplotlib to draw the figure and PyQt5 to create the GUI.

The structure of the code:



Files

doc

- SrU2F12_Raman.txt: model for the input text file containing the molecule's ideal vibration spectrum
- Yleissuunnitelma.pdf: general plan in Finnish
- Tekninen suunnitelma: technical plan in Finnish
- Raportti: project report in Finnish

src

- main.py
- gui.py: user interface
- plotfigure.py: draws the figure
- corrupted_data_file_error.py
- test.py

Instructions

- program is started by running main.py
- input spectrum is opened as a text file from the File menu: Open
- only the correct rows having two numbers are read by the program: frequency (cm^-1) and peak intensity
- figure can be adjusted by the navigation toolbar
- visibility of the computational peaks is selected with the Peaks checkbox
- the width of the peaks in the simulated spectrum can be changed with the Peak Width text field

Installation

- NumPy: "pip install numpy"
- Matplotlib: "pip install matplotlib"
- PyQt5: "pip install PyQt5"