Lorentzian_Final

November 17, 2022

1 Objective: Given a Gold nanocube, obtain its wavelength (energy) scans 10 times consecutively via AOTF-VIS. Following this:

1.0.1 1. Plot the 10 consecutive scans on a single graph, taking wavelength (nm) in the x-axis and corrected extinction (a.u) in the y-axis.

1.0.2 2. Extract the regions in all the scans where a local peak is observed. Plot them together in the same manner as above, using energy (eV) in the x-axis instead.

1.0.3 3. Obtain the best-fit Lorentzian curve for all the scans. Extract the respective Full Width at Half Maximum (FWHM) and peak Resonant Energy (E_{res}) for all of the scans. Plot all the best-fits together.

1.0.4 4. Plot all the best-fits together but ensure that the curves are normalised w.r.t. peak corrected extinction.

1.0.5 5. Obtain ΔFWHM i.e. the FWHM of all scans relative to that of the 1st scan. Plot these values w.r.t. E_{res}.

1.0.6 6. Obtain ΔE_{res} i.e. the peak Resonant Energy of all the scans relative to that of the 1st scan. Plot these values w.r.t. E_{res}.

1.0.7 7. Single-scan mode: Obtain the FWHM and E_{res} for a single scan dataset that will act as a reliability check for the entire cube.

1.1 Relevant packages and modules required

[1]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import scipy.constants as sc
import os
from pylab import cm
from lmfit.models import LorentzianModel
from tabulate import tabulate
from PIL import Image
```

1.2 Function to extract our parameters of interest as well as the number of repeats for the respective scans from the data files

[2]:
```
def parameter_formatting_WL(filename, r_skip=84, n_rows=3, loc=2):
    user_col = ["Wavelength(nm)", "FocusCorrectionY[µm]", "Repeat(x)", "M(V)",␣
 ↪"Phase(')", "IS(A)", "Phase(').1", "R(V)", "Phase(').2"]
    readfile = pd.read_csv(filename, delim_whitespace=1, skiprows=r_skip,␣
 ↪names=user_col)
    stepsfile = pd.read_csv(filename, sep='\t', skiprows=9, nrows=n_rows)
    repeats_WL = int(stepsfile.iloc[loc]['Loops:'][-8:-6])
    repeats_M = 1
    if n_rows == 4:
        repeats_M=int(stepsfile.iloc[0]['Loops:'][-9:-6])
    repeats=[repeats_WL, repeats_M]
    return readfile, repeats
```

1.3 Function to generate extinction arrays for the given csv file

[3]:
```
def extinction(readfile, repeats):
    extinctions = readfile.loc[:,"R(V)"]/readfile.loc[:,"M(V)"]
    extinctions = extinctions.groupby(np.arange(len(extinctions))//repeats[0]).
 ↪mean()
    return extinctions
```

1.4 Function to store extinction data for the consecutive scans as a 2D array i.e. Scan 1 data will be in column 1, Scan 2 in column 2, and so on

[4]:
```
def ext_matrix(extinctions, repeats):
    n_rows = len(extinctions)//repeats[1]
    n_cols = repeats[1]
    extin_matrix=np.zeros((n_rows, n_cols))
    for i in range(n_cols):
        loc = n_rows*i
        extin_matrix[:,i] = extinctions[loc:(loc+n_rows)]
    return extin_matrix
```

1.5 Function that finds the corrected extinctions for all the scans by utilising the reference data

[5]:
```
def corr_ext(extin_matrix, extin_ref):
    n_rows, n_cols = extin_matrix.shape
    corr_extin_matrix = np.zeros((n_rows, n_cols))
    for i in range(n_cols):
        corr_extin_matrix[:,i] = 1.00 - (extin_matrix[:,i]/extin_ref)
    return corr_extin_matrix
```

1.6 Function that prepares the extinction 2D array as well as the wavelengths for subsequent plotting as per Objective 1

[6]:
```
def data_prep_ob1(wavelengths, corr_extin_matrix):
    n_rows, n_cols = corr_extin_matrix.shape
    xData = np.zeros((n_cols, n_rows))
    yData = np.zeros((n_cols, n_rows))
    for i in range(n_cols):
        xData[i,:] = wavelengths
        yData[i,:] = corr_extin_matrix[:,i]
    return xData, yData
```

1.7 Function that yields the plot as per Objective 1 and 2

[7]:
```
def plot_ob1_2(xData = [], yData = [], xLabel = '', yLabel = 'Extinction (a.u.
↪)', Title = '', f = ''):
    n_rows, n_cols = yData.shape
    colors = cm.get_cmap('viridis', n_rows)
    fig = plt.figure(num = None, figsize = (10, 7), facecolor = 'w', edgecolor␣
↪= 'k')
    for i in range(n_rows):
        plt.plot(xData[i,:], yData[i,:], label = "Scan "+str(i+1), color =␣
↪colors(i))
        plt.xlabel(xLabel)
        plt.ylabel(yLabel)
        plt.legend(loc='upper right')
        plt.title(Title)
        plt.legend(bbox_to_anchor=(0.99, 0.99),  borderaxespad=0)
    #plt.show
    plt.savefig(f)
    plt.close(fig)
```

1.8 Function that converts the wavelength (in nm) to energy (in eV)

[8]:
```
def lambda_to_E(wavelengths):
    return (sc.h*sc.c*10**9/sc.e)/(wavelengths)
```

1.9 Function that yields the wavelength slice of the expected peak as well as the corresponding extinction data slice

[9]:
```
def data_slice(xData, yData, left_thres = 650.0, right_thres = 755.0):
    n_rows, n_cols = yData.shape
    xSlice = np.zeros((n_rows, n_cols))
    ySlice = np.zeros((n_rows, n_cols))
    for i in range(n_rows):
        begin_index = np.nonzero(xData[i,:] == left_thres)[0][0]
```

```
        end_index = np.nonzero(xData[i,:] == right_thres)[0][0]
        fit_range = slice(begin_index, end_index+1)
        xSlice[i,fit_range] = xData[i,fit_range]
        ySlice[i,fit_range] = yData[i,fit_range]
    return xSlice[:, ~np.all(xSlice == 0, axis = 0)], ySlice[:, ~np.all(ySlice␣
↪== 0, axis = 0)]
```

1.10 Function that obtains the best-fit Lorentzian curves for the consecutive data slices provided

[10]:
```
def lorentzian_fit(xSlice, ySlice):
    n_rows, n_cols = ySlice.shape
    model = LorentzianModel()
    result_params = []
    result_bestfit = np.zeros((n_rows, n_cols))
    for i in range(n_rows):
        params = model.guess(ySlice[i,:], xSlice[i,:])
        results = model.fit(ySlice[i,:], params, x=xSlice[i,:])
        result_params.append(list(results.params.items()))
        result_bestfit[i,:] = results.best_fit
    return result_params, result_bestfit
```

1.11 Function that extracts the model best-fit parameters held in a dictionary and stores it in a 2D array

[11]:
```
def param_dict_array(params):
    n_rows = len(params)
    no_of_params = len(params[0])
    param_set = np.zeros((n_rows, no_of_params))
    for i in range(n_rows):
        for j in range(no_of_params):
            param_set[i,j] = params[i][j][1].value
    return param_set
```

1.12 Function that extracts the FWHM, E_{res}, and height of peak maxima for the 10 consecutive scans

[12]:
```
def param_extract(param_set):
    E_res = param_set[:,1]
    fwhm = param_set[:,3]
    height_max_peak = param_set[:,4]
    return fwhm, E_res, height_max_peak
```

1.13 Function that tabulates the FWHM, ΔFWHM, E_{res}, ΔE_{res}, and Height of peak maxima for the 10 consecutive scans

[13]:
```
def param_table(fwhm, delta_fwhm, E_res, delta_E_res, h_max, f):
    num_el = len(fwhm)
    table = np.zeros((num_el,6))
    col_names = ['Scan no.', 'FWHM (eV)', 'ΔFWHM (meV)', 'E_res (eV)', 'ΔE_res␣
↪(meV)', 'h_peak (a.u.)']
    for i in range(num_el):
        table[i,:] = [i+1, fwhm[i], delta_fwhm[i]*1000, E_res[i],␣
↪delta_E_res[i]*1000, h_max[i]]
    #print(tabulate(table, headers='firstrow', tablefmt='fancy_grid',␣
↪floatfmt=".4f"))
    table_df1 = pd.DataFrame(table, columns = col_names)
    table_df = table_df1.copy()
    table_df.update(table_df.applymap('{:,.4f}'.format))
    table_df['Scan no.'] = table_df['Scan no.'].astype(float).astype(int)
    plt.rcParams["figure.figsize"] = [10, 7]
    plt.rcParams["figure.autolayout"] = True
    fig, ax = plt.subplots()
    fig.patch.set_visible(False)
    ax.axis('off')
    ax.axis('tight')
    table_fig = ax.table(cellText = table_df.convert_dtypes().to_numpy(),␣
↪colLabels = table_df.columns,
                         colWidths = [0.1, 0.18, 0.18, 0.18, 0.18, 0.18],␣
↪loc='center', cellLoc='center')
    table_fig.scale(1, 1.5)
    table_fig.auto_set_font_size(False)
    table_fig.set_fontsize(8)
    fig.tight_layout()
    plt.savefig(f.replace('.csv','.png').replace('/csv/','/Figures/'), dpi =␣
↪300)
    plt.close(fig)
    table_df1.to_csv(f, index=False, header=False)
```

1.14 Function that normalizes the extinction dataset as well as the best-fit extinction dataset w.r.t. height of peak maxima for the 10 consecutive scans as per Objective 4

[14]:
```
def extinction_normalize(yData, yFit, h_max):
    n_rows, n_cols = yData.shape
    yData_norm = np.zeros((n_rows, n_cols))
    yFit_norm = np.zeros((n_rows, n_cols))
    for i in range(n_rows):
        yData_norm[i,:] = yData[i,:]/h_max[i]
```

```
        yFit_norm[i,:] = yFit[i,:]/h_max[i]
    return yData_norm, yFit_norm
```

1.15 Function that plots the best-fit Lorentzian curves along with the corresponding datasets (as dots) for the 10 consecutive scans as per Objective 3 and 4

[15]:
```
def plot_ob3_4(xData = [], yData = [], yFit = [], xLabel = '', yLabel =␣
 ↪'Extinction (a.u.)', Title = '', f = ''):
    n_rows, n_cols = yData.shape
    colors = cm.get_cmap('viridis', n_rows)
    fig = plt.figure(num = None, figsize = (10, 7), facecolor = 'w', edgecolor␣
 ↪= 'k')
    for i in range(n_rows):
        plt.plot(xData[i,:], yFit[i,:], '-', label = "Scan "+str(i+1), color =␣
 ↪colors(i))
        plt.plot(xData[i,:], yData[i,:], '.', color = colors(i))
        plt.xlabel(xLabel)
        plt.ylabel(yLabel)
        plt.legend(loc='upper right')
        plt.title(Title)
        plt.legend(bbox_to_anchor=(0.99, 0.99),  borderaxespad=0)
    #plt.show
    plt.savefig(f)
    plt.close(fig)
```

1.16 Function that finds ΔFWHM and ΔE_{res} as per Objective 5 and 6

[16]:
```
def delta_param(fwhm, E_res):
    n_rows = len(fwhm)
    delta_fwhm = []
    delta_E_res = []
    for i in range(n_rows):
        delta_fwhm.append((fwhm[i] - fwhm[0]))
        delta_E_res.append((E_res[i] - E_res[0]))
    return delta_fwhm, delta_E_res
```

1.17 Function that plots ΔFWHM (meV) and ΔE_{res} (meV) versus E_{res} (eV) for the 10 consecutive scans as per Objective 5 and 6

[17]:
```
def plot_ob5_6(xData = [], yData = [], xLabel = '', yLabel = '', Title = '', f␣
 ↪= '', loci = 'best'):
    n_rows = len(yData)
    colors = cm.get_cmap('viridis', n_rows)
    fig = plt.figure(num = None, figsize = (10, 7), facecolor = 'w', edgecolor␣
 ↪= 'k')
```

```
    for i in range(n_rows):
        plt.plot(xData[i], yData[i]*1000, '.', label = "Scan "+str(i+1), color␣
↪= colors(i))
        plt.xlabel(xLabel)
        plt.ylabel(yLabel)
        plt.legend(loc=loci)
        plt.title(Title)
        #plt.legend(bbox_to_anchor=(0.99, 0.99),  borderaxespad=0)
    #plt.show
    plt.savefig(f)
    plt.close(fig)
```

1.18 Function that tabulates the ΔFWHM (meV) and ΔE_{res} (meV) for the 10th scan

[18]:
```
def scan10_table(delta_fwhm, delta_E_res, f):
    table = [delta_fwhm[-1]*1000, delta_E_res[-1]*1000]
    #print(tabulate(table, headers='firstrow', tablefmt='fancy_grid',␣
↪floatfmt=".4f"))
    table_df1 = pd.DataFrame([table], columns = ['ΔFWHM_cube (meV)',␣
↪'ΔE_res_cube (meV)'])
    table_df = table_df1.copy()
    table_df.update(table_df.applymap('{:,.4f}'.format))
    plt.rcParams["figure.figsize"] = [10, 7]
    plt.rcParams["figure.autolayout"] = True
    fig, ax = plt.subplots()
    fig.patch.set_visible(False)
    ax.axis('off')
    ax.axis('tight')
    table_fig = ax.table(cellText = table_df.values, colLabels = table_df.
↪columns, loc='center', cellLoc='center')
    table_fig.scale(1, 2)
    table_fig.set_fontsize(16)
    fig.tight_layout()
    plt.savefig(f.replace('.csv','.png').replace('/csv/','/Figures/'), dpi =␣
↪300)
    plt.close(fig)
    table_df1.to_csv(f, index=False, header=False)
```

1.19 Function that tabulates the FWHM and E_{res} for single scan mode as per Objective 7

[19]:
```
def scan1_table(fwhm, E_res, f):
    table = [fwhm[0], E_res[0]]
    #print(tabulate(table, headers='firstrow', tablefmt='fancy_grid',␣
↪floatfmt=".4f"))
```

```python
    table_df1 = pd.DataFrame([table], columns = ['FWHM (eV)', 'E_res (eV)'])
    table_df = table_df1.copy()
    table_df.update(table_df.applymap('{:,.4f}'.format))
    plt.rcParams["figure.figsize"] = [10, 7]
    plt.rcParams["figure.autolayout"] = True
    fig, ax = plt.subplots()
    fig.patch.set_visible(False)
    ax.axis('off')
    ax.axis('tight')
    table_fig = ax.table(cellText = table_df.values, colLabels = table_df.
↪columns, loc='center', cellLoc='center')
    table_fig.scale(1, 2)
    table_fig.set_fontsize(16)
    fig.tight_layout()
    plt.savefig(f.replace('.csv','.png').replace('/csv/','/Figures/'), dpi =␣
↪300)
    plt.close(fig)
    table_df1.to_csv(f, index=False, header=False)
```

1.20 Function that generates a PDF report of all the plots and tables obtained for the given scan

[20]:
```python
def get_report(cwd, fig_dir, csv_dir, export_list, f, dpi = 300):
    num_el = len(export_list)
    png_index = []
    csv_index = []
    for i in range(num_el):
        if export_list[i][-4:None] == '.png':
            png_index.append(i)
        elif export_list[i][-4:None] == '.csv':
            csv_index.append(i)
        else:
            continue
    images = []
    wanted_dpi = dpi
    for i in png_index:
        images.append(Image.open(cwd + fig_dir + export_list[i]))
    for i in csv_index:
        images.append(Image.open(cwd + fig_dir + export_list[i].replace('.
↪csv','.png')))
    image_rgb = []
    for img in images:
        try:
            dpi_x, dpi_y = img.info["dpi"]
        except KeyError:
            dpi_x, dpi_y = dpi, dpi
```

```
        dpi_x_resize = round(img.width*wanted_dpi/dpi_x)
        dpi_y_resize = round(img.height*wanted_dpi/dpi_y)
        img = img.resize((dpi_x_resize, dpi_y_resize), resample=Image.LANCZOS)
        img_rgb = Image.new('RGB', img.size, (255, 255, 255))
        img_rgb.paste(img, mask = img.split()[3])
        image_rgb.append(img_rgb)
    pdf_path = cwd + '/' + f
    image_rgb[0].save(pdf_path, "PDF" ,resolution=100.0, optimize=True,␣
 ↪save_all=True, append_images=image_rgb[1:])
```

1.21 Function where the protocol is executed for all objectives

[21]:
```
def Nanocube_Lorentzian(mode, f1, f2, title_list, export_list):

    cwd = os.getcwd()
    csv_dir = '/csv/'
    fig_dir = '/Figures/'

    if mode == 1:
        hits, repeats1 = parameter_formatting_WL(cwd + csv_dir + f1, 84, 3, 2)
    else:
        hits, repeats1 = parameter_formatting_WL(cwd + csv_dir + f1, 86, 4, 3)

    miss, repeats2 = parameter_formatting_WL(cwd + csv_dir + f2, 84, 3, 2)

    hits_ext = extinction(hits, repeats1)
    miss_ext = extinction(miss, repeats2)

    hits_ext_matrix = ext_matrix(hits_ext, repeats1)

    corr_hits_ext_matrix = corr_ext(hits_ext_matrix, miss_ext)

    wavelengths = miss.loc[::repeats2[0],'Wavelength(nm)'].values

    xdata, ydata = data_prep_ob1(wavelengths, corr_hits_ext_matrix)

    plot_ob1_2(xdata, ydata, 'Wavelength (nm)', 'Extinction (a.u.)',␣
 ↪title_list[0], cwd + fig_dir + export_list[0])

    xslice1, yslice = data_slice(xdata, ydata)
    xslice = lambda_to_E(xslice1)

    plot_ob1_2(xslice, yslice, 'Energy (eV)', 'Extinction (a.u.)',␣
 ↪title_list[1], cwd + fig_dir + export_list[1])

    fit_params, fit_ydata = lorentzian_fit(xslice, yslice)
```

```
    fit_param_set = param_dict_array(fit_params)

    FWHM, E_res, height_max_peak = param_extract(fit_param_set)

    plot_ob3_4(xslice, yslice, fit_ydata, 'Energy (eV)', 'Extinction (a.u.)',␣
↪title_list[2], cwd + fig_dir + export_list[2])
    plot_ob1_2(xslice, fit_ydata, 'Energy (eV)', 'Extinction (a.u.)',␣
↪title_list[3], cwd + fig_dir + export_list[3])

    yslice_norm, fit_ydata_norm = extinction_normalize(yslice, fit_ydata,␣
↪height_max_peak)

    plot_ob3_4(xslice, yslice_norm, fit_ydata_norm, 'Energy (eV)', 'Extinction␣
↪(a.u.)', title_list[4], cwd + fig_dir + export_list[4])
    plot_ob1_2(xslice, fit_ydata_norm, 'Energy (eV)', 'Extinction (a.u.)',␣
↪title_list[5], cwd + fig_dir + export_list[5])

    if mode == 1:
        scan1_table(FWHM, E_res, cwd + csv_dir + export_list[6])
        get_report(cwd, fig_dir, csv_dir, export_list, 'Single_scan_report.pdf')
    else:
        delta_FWHM, delta_E_res = delta_param(FWHM, E_res)

        plot_ob5_6(E_res, delta_FWHM, 'E_res (eV)', 'ΔFWHM (meV)',␣
↪title_list[6], cwd + fig_dir + export_list[6])
        plot_ob5_6(E_res, delta_E_res, 'E_res (eV)', 'ΔE_res (meV)',␣
↪title_list[7], cwd + fig_dir + export_list[7], 'lower right')

        param_table(FWHM, delta_FWHM, E_res, delta_E_res, height_max_peak, cwd␣
↪+ csv_dir + export_list[8])
        scan10_table(delta_FWHM, delta_E_res, cwd + csv_dir + export_list[9])
        get_report(cwd, fig_dir, csv_dir, export_list, 'Consecutive_scan_report.
↪pdf')
```

1.22 Main function for Consecutive Scans Mode

[22]:
```
def Consecutive_Scans_Mode(f1 = "10ConsScan_cube9.csv", f2 =␣
↪"10ConsScan_cube9ref.csv"):

    title_list = ['','','','','','','','']
    export_list = ['','','','','','','','','','']

    title_list[0] = 'Consecutive Wavelength Scans on Nanocube'
    title_list[1] = 'Consecutive Wavelength Scans on Nanocube'
    title_list[2] = 'Best-fit Lorentzian Curves for Consecutive Scans'
    title_list[3] = 'Best-fit Lorentzian Curves for Consecutive Scans'
```

```
    title_list[4] = 'Normalized Best-fit Lorentzian Curves for Consecutive␣
↪Scans'
    title_list[5] = 'Normalized Best-fit Lorentzian Curves for Consecutive␣
↪Scans'
    title_list[6] = 'Change in FWHM vs E_res'
    title_list[7] = 'Change in E_res vs E_res'

    export_list[0] = 'Full_wavelength_scan.png'
    export_list[1] = 'Sliced_energy_scan.png'
    export_list[2] = 'Best-fit_Lorentzian_with_dataset.png'
    export_list[3] = 'Best-fit_Lorentzian.png'
    export_list[4] = 'Best-fit_Lorentzian_with_dataset_normalized.png'
    export_list[5] = 'Best-fit_Lorentzian_normalized.png'
    export_list[6] = 'Delta_FWHM_vs_E-res.png'
    export_list[7] = 'Delta_E-res_vs_E-res.png'
    export_list[8] = 'Parameters_of_interest.csv'
    export_list[9] = 'Cube_parameters.csv'

    Nanocube_Lorentzian(2, f1, f2, title_list, export_list)
```

1.23 Main function for Single Scan mode

[23]:
```
def Single_Scan_Mode(f1 = "C5.csv", f2 = "C5_ref.csv"):

    title_list = ['','','','','','']
    export_list = ['','','','','','','']

    title_list[0] = 'Single Wavelength Scan on Nanocube'
    title_list[1] = 'Single Wavelength Scan on Nanocube'
    title_list[2] = 'Best-fit Lorentzian Curve for Single Scan'
    title_list[3] = 'Best-fit Lorentzian Curve for Single Scan'
    title_list[4] = 'Normalized Best-fit Lorentzian Curve for Single Scan'
    title_list[5] = 'Normalized Best-fit Lorentzian Curve for Single Scan'

    export_list[0] = 'Single_wavelength_scan.png'
    export_list[1] = 'Single_Sliced_energy_scan.png'
    export_list[2] = 'Single_Best-fit_Lorentzian_with_dataset.png'
    export_list[3] = 'Single_Best-fit_Lorentzian.png'
    export_list[4] = 'Single_Best-fit_Lorentzian_with_dataset_normalized.png'
    export_list[5] = 'Single_Best-fit_Lorentzian_normalized.png'
    export_list[6] = 'Single_scan_parameters.csv'

    Nanocube_Lorentzian(1, f1, f2, title_list, export_list)
```

1.24 Main function that takes in the Mode type as input:

1.24.1 1. Single Scan Mode → Enter 1

1.24.2 2. Consecutive Scans Mode → Enter 2

[24]:
```
def main_func(mode):
    if mode == 1:
        Single_Scan_Mode()
    elif mode == 2:
        Consecutive_Scans_Mode()
    else:
        print("Invalid input")
        return None
```

1.25 Just call the main function!

[25]:
```
main_func(1)
```

[26]:
```
main_func(2)
```