EDRIXS_compare_new_funcs.

February 27, 2022

[1]:
```
%matplotlib inline
```

[2]:
```
import edrixs
import numpy as np
import lmfit
import matplotlib.pyplot as plt
import io
import sys
from ana_functions import *
from scipy.signal import find_peaks

%matplotlib inline
```

Confirm consistency of new function, in which transitions have specifically specified width, and original EDRIXS

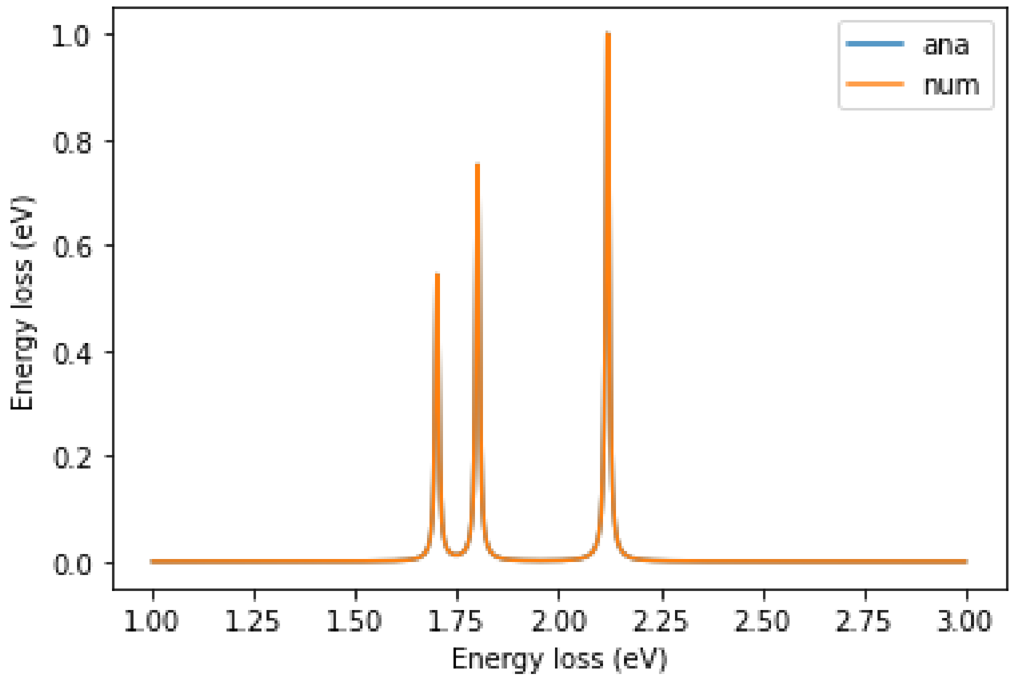
[3]:
```
Ez2 = 1.7 # 1.7
Exy = 1.8
Ezx = 2.12 #2.12

Wz2 = 0.01
Wxy = 0.01
Wx2y2 = 0.01
Wzx = 0.01

J = .130*0

res = 1e-9

alpha = np.pi/2 # rad
thin = 45       # deg
thout = 45     # deg
phi = 0        # deg

eloss = np.linspace(1, 3, 1000000)

orbital_index_i = 3
spin_index_i = 0
```

```python
Iana = get_RIXS(eloss,
             Ez2=Ez2, Ezx=Ezx, Exy=Exy,
             Wz2=Wz2, Wzx=Wzx, Wxy=Wxy,
             J=J, res=res,
             I0=1,
             thin=thin, thout=thout, phi=phi,
             alpha=alpha,
             select=range(5))

# Standard EDRIXS here
pol_type_rixs = [('linear', alpha, 'linear', 0), ('linear', alpha, 'linear', np.
 ↪pi/2)]

shell_name = ('d', 'p32')
v_noccu = 9
off = 931

ext_B = np.array([1e-4, 1e-4, 0])
temperature = 1e-9

# d3z2-r2 dzx dzy dx2-y2 dxy
tmp = np.array([-en for dd in [Ez2, Ezx, Ezx, 0, Exy] for en in [dd]*2])
v_cfmat = edrixs.cb_op(np.diag(tmp), edrixs.tmat_r2c('d', ispin=True))

info = edrixs.utils.get_atom_data('Cu', '3d', v_noccu, edge='L3')
v_soc = None
c_soc = info['c_soc']


out = edrixs.ed_1v1c_py(shell_name, shell_level=(0, -off), v_soc=v_soc,
                        c_soc=c_soc, v_noccu=v_noccu,
                        ext_B=ext_B, on_which='spin', v_cfmat=v_cfmat)
eval_i, eval_n, trans_op = out

ominc = np.linspace(925, 935, 2000)

xas = edrixs.xas_1v1c_py(
    eval_i, eval_n, trans_op, ominc, gamma_c=info['gamma_c'],
    thin=0, phi=0, pol_type=[('isotropic', 0)])

res_energy = ominc[np.argmax(xas[:, 0])]
assert res_energy > 926
assert res_energy < 934

                    #(x, center, amplitude, width, offset)
gamma_f = Wz2/2 # lorentzian HWHM
```

```
rixs = edrixs.rixs_1v1c_py(
    eval_i, eval_n, trans_op, [res_energy], eloss,
    gamma_c=info['gamma_c'], gamma_f=gamma_f,
    thin=thin*np.pi/180, thout=thout*np.pi/180, phi=phi*np.pi/180,
    pol_type=pol_type_rixs, gs_list=[0, 1],
    temperature=temperature
    )

I_num=rixs.sum((0, 2))

fig, ax = plt.subplots()

ax.plot(eloss, Iana/Iana.max(), label='ana')
ax.plot(eloss, I_num/I_num.max(), label='num')
ax.set_xlabel('Energy loss (eV)')
ax.set_ylabel('Energy loss (eV)')
ax.legend()
```

```
edrixs >>> Running ED …

    Summary of Slater integrals:
    ------------------------------
    Terms,   Initial Hamiltonian,  Intermediate Hamiltonian
     F0_vv :          0.0000000000        0.0000000000
     F2_vv :          0.0000000000        0.0000000000
     F4_vv :          0.0000000000        0.0000000000
     F0_vc :          0.0000000000        0.0000000000
     F2_vc :          0.0000000000        0.0000000000
     G1_vc :          0.0000000000        0.0000000000
     G3_vc :          0.0000000000        0.0000000000
     F0_cc :          0.0000000000        0.0000000000
     F2_cc :          0.0000000000        0.0000000000

edrixs >>> Dimension of the initial Hamiltonian:  10
edrixs >>> Dimension of the intermediate Hamiltonian:  4
edrixs >>> Building Many-body Hamiltonians …
edrixs >>> Done !
edrixs >>> Exact Diagonalization of Hamiltonians …
edrixs >>> Done !
edrixs >>> ED Done !
edrixs >>> Running XAS …
edrixs >>> XAS Done !
edrixs >>> Running RIXS …
edrixs >>> RIXS Done !
```

[3]:
```
<matplotlib.legend.Legend at 0x7f2139f457b8>
```



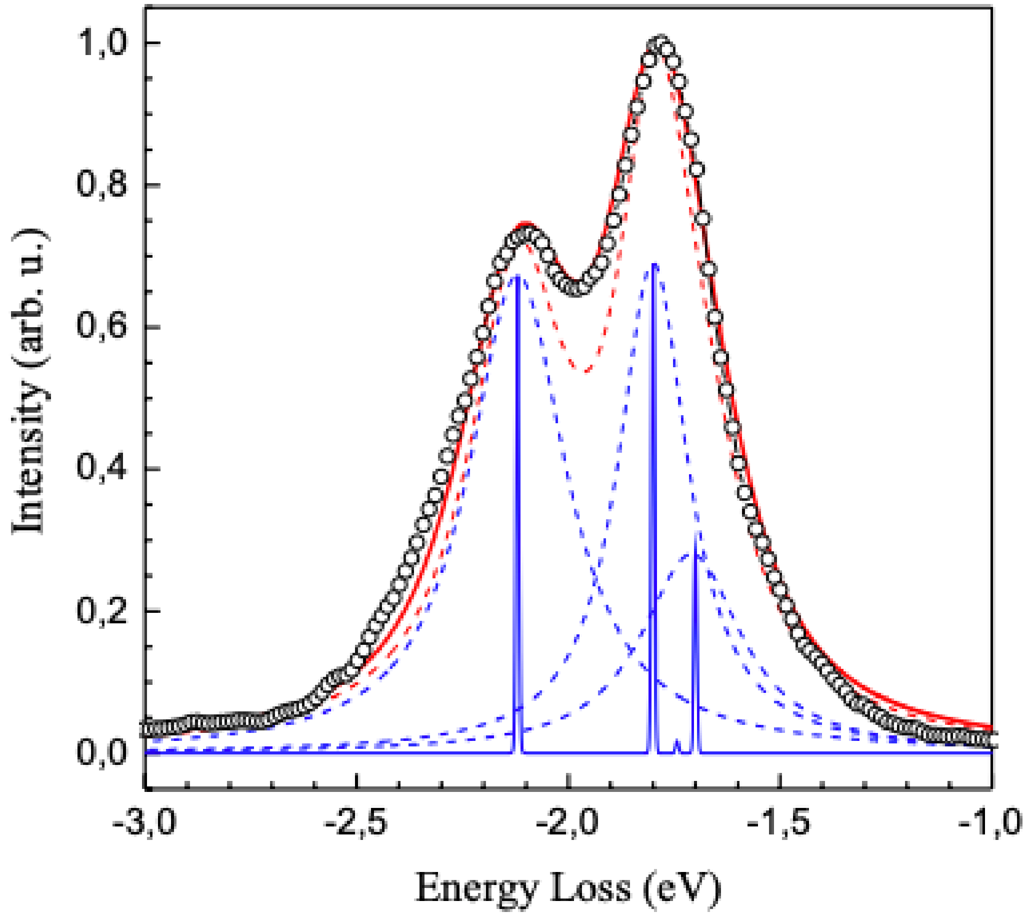
[4]:
```
indices = find_peaks(Iana/Iana.max(), height=.1)
indices
```

[4]:
```
(array([350000, 399999, 559999]),
 {'peak_heights': array([0.54356914, 0.75141954, 1.        ])})
```

Why is this not the same as M. Moretti et al., New Journal of Physics 13, 043026 (2011) Fig. 4? The very small peak in the Moretti plot comes from an orbital-dependent exchange splitting that cannot easily be put into standard edixs, but which is not the source of the discrepancy.

[5]:
```
from IPython.display import Image
Image(filename='moretti.png')
```

[5]:


Intensity (arb. u.)
1,0
0,8
0,6
0,4
0,2
0,0
-3,0
-2,5
-2,0
-1,5
-1,0
Energy Loss (eV)

[ ]: