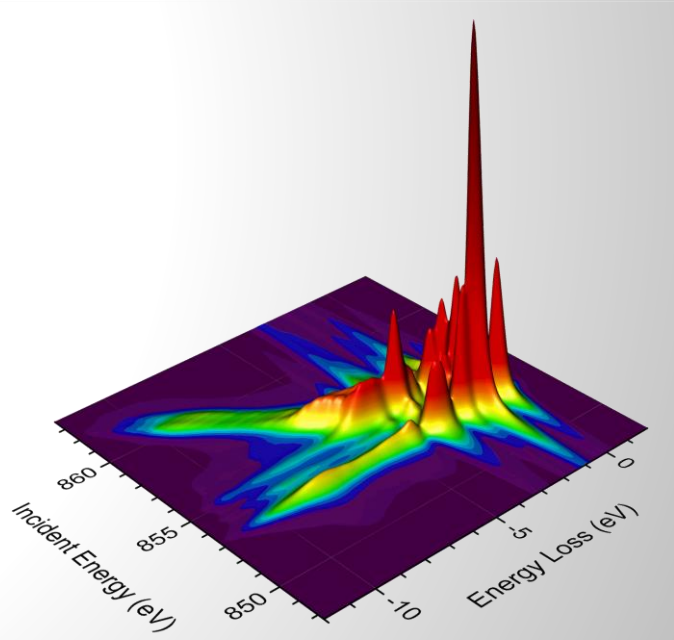
Analysis of soft XAS and RIXS with multiplet models using Quanty

Part 1: Understanding the Spectra

Part 2: Quanty Computations



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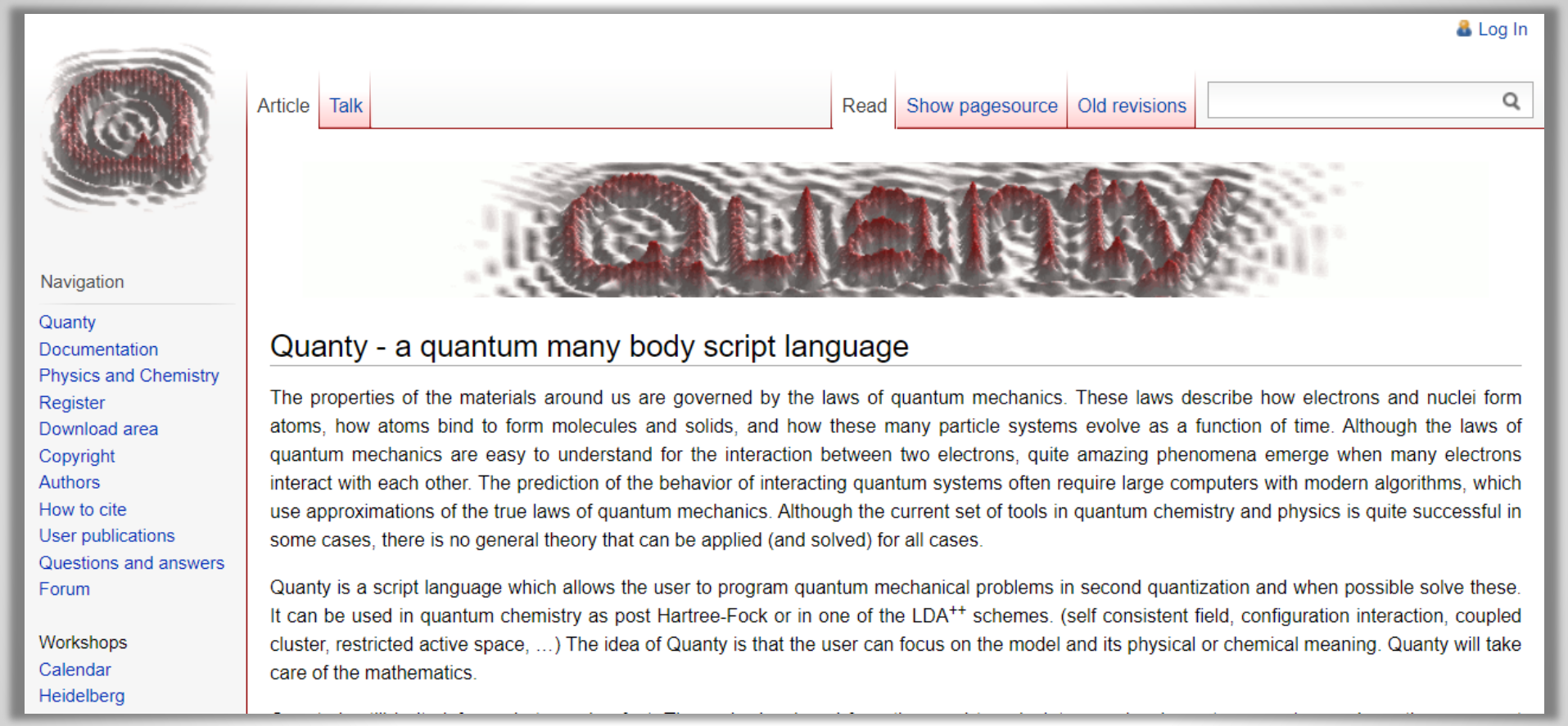
https://quanty.org



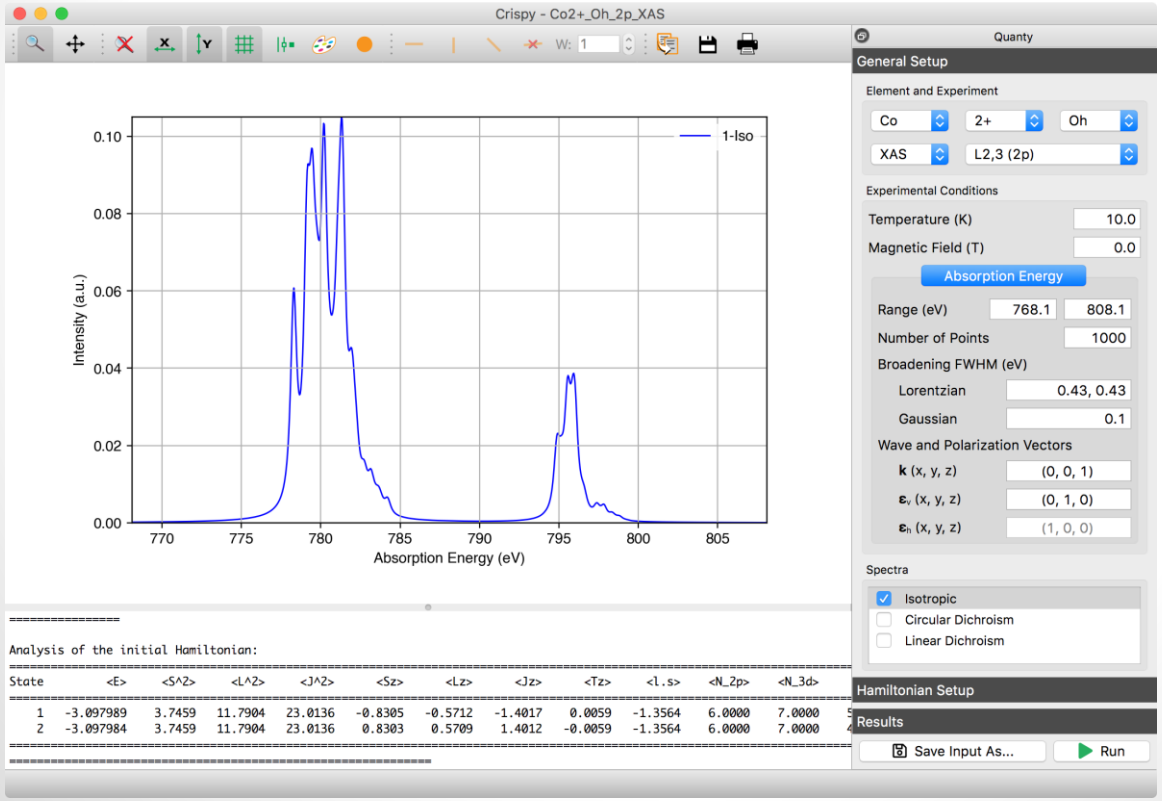
Lots of information on the website

– installation, execution, tutorials/examples, and full documentation of all capabilities

Quanty is designed as an executable program that reads input files written in the Lua scripting language. This makes it extremely flexible and powerful.

However, a 3rd party graphical user interface called Crispy has been written for Quanty, which works well for many standard types of calculations

https://www.esrf.fr/computing/scientific/crispy/index.html



A Typical Quanty Computation

Define a Hamiltonian (H) operator to model your system

```
H =  F0dd*OppF0_3d + F2dd*OppF2_3d + F4dd*OppF4_3d
```

The majority of the work

Compute some eigenstates of this H

```
psiList = Eigensystem(H, StartRestrictions, Npsi)
```

Compute properties for the eigenstates of this H

```
E0 = psiList[1]*H*psiList[1]
```

$$E_0 = \langle \Psi_0 | H | \Psi_0 \rangle$$

Compute XAS spectra for this H

```
XASSpectra = CreateSpectra(XASH, T2p3dx, psiList[1], {{ ...
```

Compute RIXS spectra for this H

```
RIXSSpectra = CreateResonantSpectra(XASH, H, T2p3dx, T3d2py, psiList[1], { ...
```

Calculations of NiO with Increasing Complexity

NiO is a good example, as simple models like crystal field theory do well, but we can also see definite improvements when going all the way to high complexity impurity models

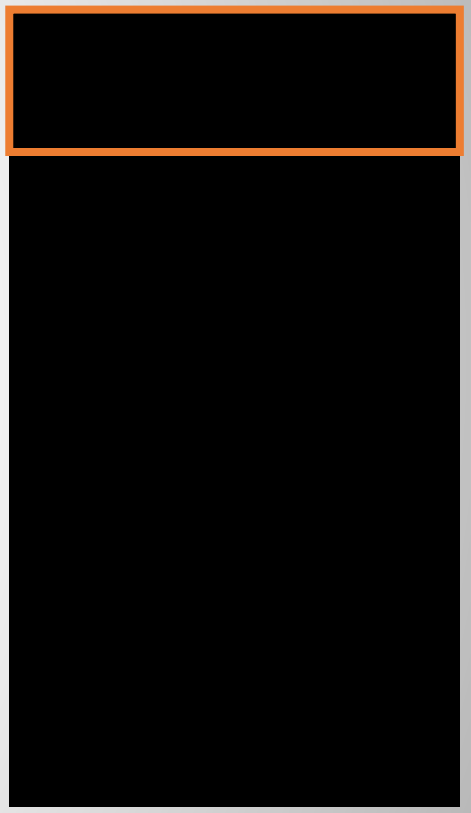
In this example, we'll learn how to compute NiO XAS and RIXS for three of the models discussed in Part 1:

- atomic model
- crystal field model
- ligand field model

Anatomy of a Typical Quanty File

Define orbital indices:

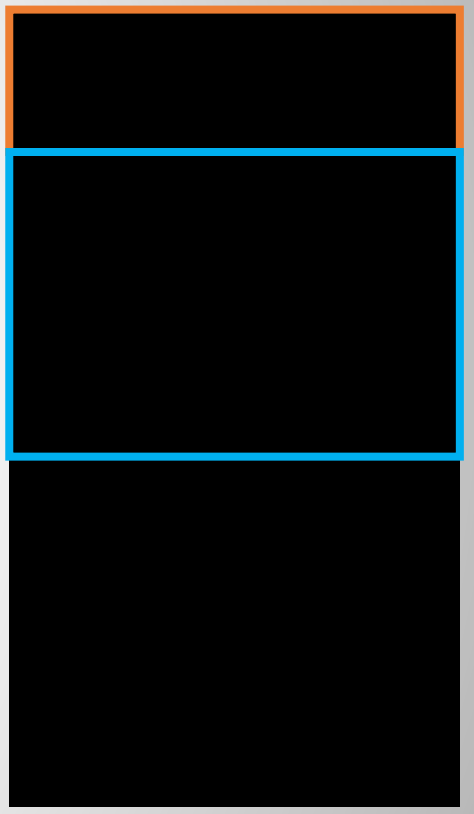
```
NF=28
NB=0
IndexDn_2p={ 0, 2, 4}
IndexUp_2p={ 1, 3, 5}
IndexDn_3s={ 6}
IndexUp_3s={ 7}
IndexDn_3d={ 8,10,12,14,16}
IndexUp_3d={ 9,11,13,15,17}
IndexDn_Ld={18,20,22,24,26}
IndexUp_Ld={19,21,23,25,27}
```



Anatomy of a Typical Quanty File

Define operators:

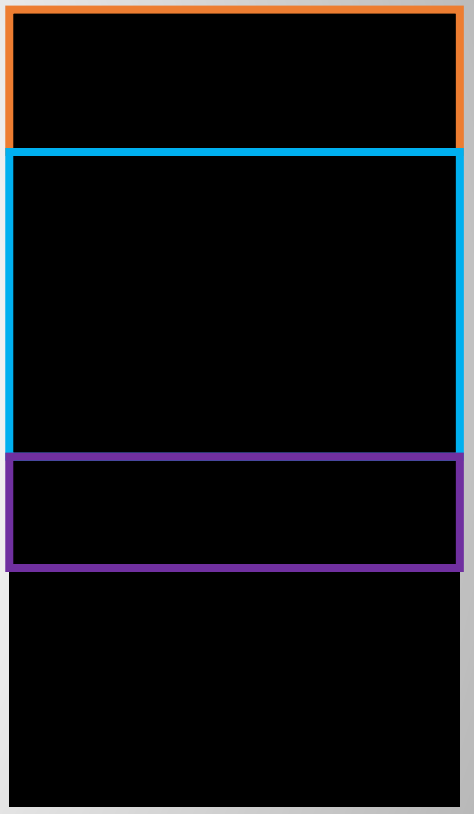
```
Akm = PotentialExpandedOnClm("Oh", 2, {0.6,-0.4})
Akm = PotentialExpandedOnClm("Oh", 2, {1,0})
Akm = PotentialExpandedOnClm("Oh", 2, {0,1})

OpptenDq_3d = NewOperator("CF", NF, IndexUp_3d, IndexDn_3d, Akm)
OppNeg_3d   = NewOperator("CF", NF, IndexUp_3d, IndexDn_3d, Akm)
OppNt2g_3d  = NewOperator("CF", NF, IndexUp_3d, IndexDn_3d, Akm)
```



Anatomy of a Typical Quanty File

Define scalar parameters:

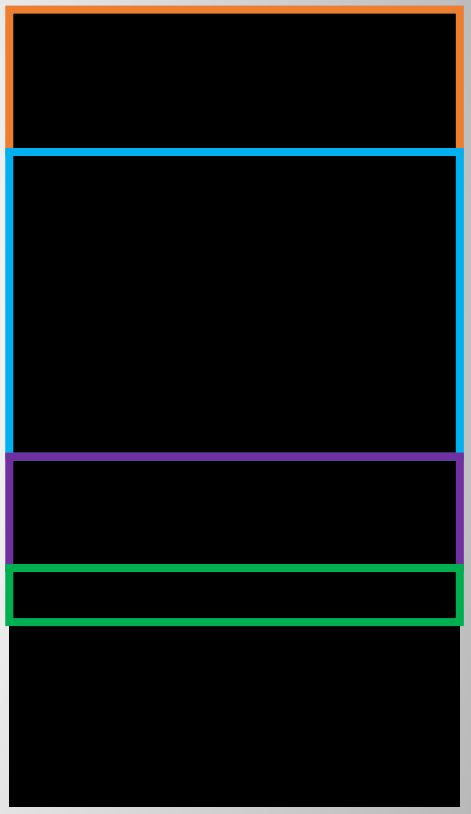
```
nd = 8

Udd     =  7.3
Upd     =  8.5
Delta   =  4.7

F2dd    = 11.14
F4dd    =  6.87
F2pd    =  6.67
G1pd    =  4.92
G3pd    =  2.80

tenDq   =  0.56

Veg     =  2.06
Vt2g    =  1.21

zeta_3d =  0.081
zeta_2p = 11.51
```



Anatomy of a Typical Quanty File

Construct Hamiltonian:

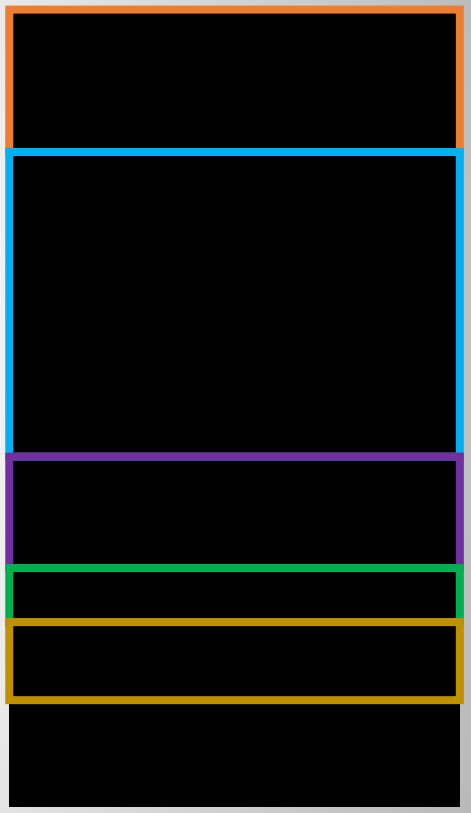
```
H =  F0dd*OppF0_3d +
     F2dd*OppF2_3d +
     F4dd*OppF4_3d +
     zeta_3d*Oppldots_3d +
     Bz*(2*OppSz_3d + OppLz_3d) +
     tenDq*OpptenDq_3d +
     tenDqL*OpptenDq_Ld +
     Veg * OppVeg +
     Vt2g * OppVt2g +
     ed * OppN_3d +
     eL * OppN_Ld
```



Anatomy of a Typical Quanty File

Calculate ground state and expectation values:

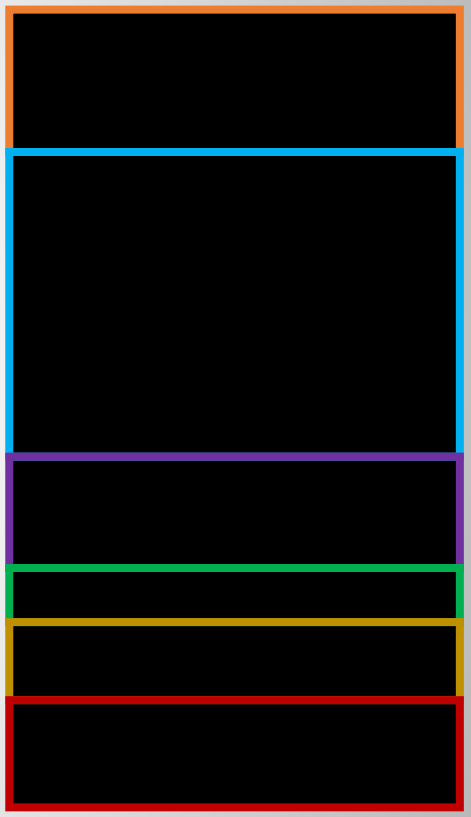
```
psiList = Eigensystem(Hamiltonian, StartRestrictions, Npsi)

print("E0:  ", psiList[1]*H*psiList[1])
print("N3d: ", psiList[1]*OppN_3d*psiList[1])
print("S^2: ", psiList[1]*OppSsqr*psiList[1])
```



Anatomy of a Typical Quanty File

Calculate spectra and save to file:

```
XASSpectra = CreateSpectra(XASHamiltonian, T2p3dx, psiList[1],
            {{"Emin",-10}, {"Emax",20}, {"NE",3500}, {"Gamma",0.45}})

XASSpectra.Broaden(0,0.3)
XASSpectra.Print({{"file", "RIXSL23M45_XAS.dat"}})
```



[Live Demo]

Concluding Remarks

Input files for the cases discussed today are available

Many more tutorials on Quanty website

Quanty workshops are held on an almost annual basis: https://quanty.org/workshop/start

There is a Quanty help forum: https://quanty.org/forum/start

Quanty is a great tool to learn about quantum mechanics (but you also don't need to know QM, for example if using Crispy)

Common pitfall: adjusting parameters to unfeasible values

- Compare charge transfer and hybridization parameters to established works on similar materials
- Are crystal field energies reasonable, given the structure of your material?
- Are your Slater integrals reasonable, given the element and oxidation state?
- Are the eigenstate properties comparable to expectations?
    - i.e. have other works determined spin state, electron occupations, etc?

Good reference: "Core Level Spectroscopy of Solids", Frank de Groot and Akio Kotani, CRC Press (2008)