Walkthrough for the K-K Transform Functions:

kkXANES(), kkImag(), and kkReal()

By Zachary Porter

SSRL MSD Hard X-rays

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1) **It's all at: 'P:\bl2-1\ZP\KK_Transform\'**

2) **Purpose**

   This code was written to perform a KK transform as a black box operation.

   It handles most of the details behind the scenes (like dealing with poorly spaced energy values), is meant to be resistant to errors, and can work with minimal inputs.

   It is well commented and hopefully easy to debug and modify for future applications.

3) **The code's help sections are better than this.**

   I maintained clear descriptions in the files named above.

4) **Preparing the inputs**

   a. <u>Starting from XANES</u>

      kkXANES() is meant for normalized, background-subtracted XANES from a program like Sixpack. Please remove all strings prior to the lines of numerical data, and make the energies into one array and the μ(E) as another. *kkXANES()* should solve for both f'' (directly by fitting) and f' (as a KK transform of f'').

b. Starting from scattering factors

Alternatively, if you are starting with f’ and f’’, from a GenX fit for instance, then you should immediately use *kkReal()* or *kkImag()*.

5) Function Calls

a. Minimum inputs

kk_() functions can all be called with three inputs:

1st the double array to transform,

2nd the double array of corresponding energies, and

3rd the string of the element name with the absorption edge of interest

The default is to NOT show plots and to NOT subtract Z from f’ input data

b. Other inputs

The next (optional) input allows you to specify the Energy region of interest, E_ROI

It is a 1x2 vector of the bounds, in eV

By default it is [E_low+100, E_high+100], if left empty

The next inputs are Booleans. In order, they are:

1 to show plots (time-consuming!!!!)

1 to subtract Z from f’ inputs (only applicable to *kkImag()*)

6) Outputs

a. Minimum Outputs

For *kkReal()*,the 1st output will be f’ for the input energy values E_given

For *kkImag()*, it is the same (but f’’)

For *kkXANES()*, it is both (f’ then f’’)

b. Other outputs

This code has a variable number of outputs.

Read the documentation for information on the outputs.

In general they are the input spliced into the widest possible energy range (typically 20eV to 400keV), along with this energy range, and then the FULL KK transform of the input over this energy range. This last input is very time-consuming to compute so I advise against it unless totally necessary.

c. Energy Step Clarification

The steps in energy are decided from the input data. Before the input data are transformed they are interpolated to an evenly spaced energy grid. The spacing on this grid is either 0.5eV steps or the smallest energy step in the input data, whichever is larger.

7) Example

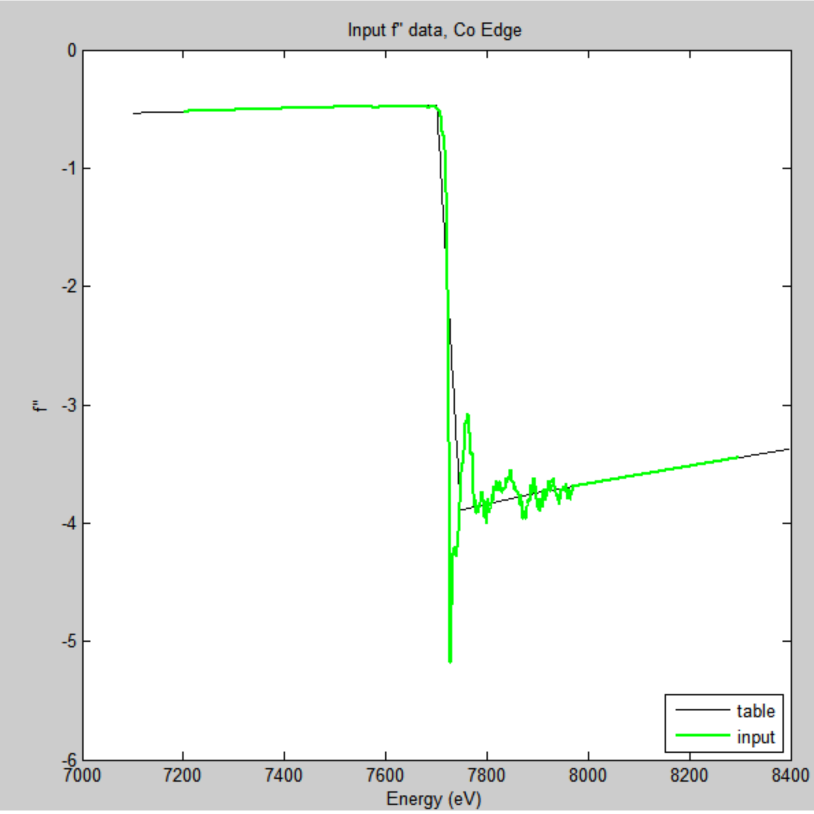
a. Load some f’, f’’ data calculated from XANES, the ‘kk_example_data.mat’ file (calling the arrays ref, imf, and E; note this is Co data from sample X11)

b. Call the function:

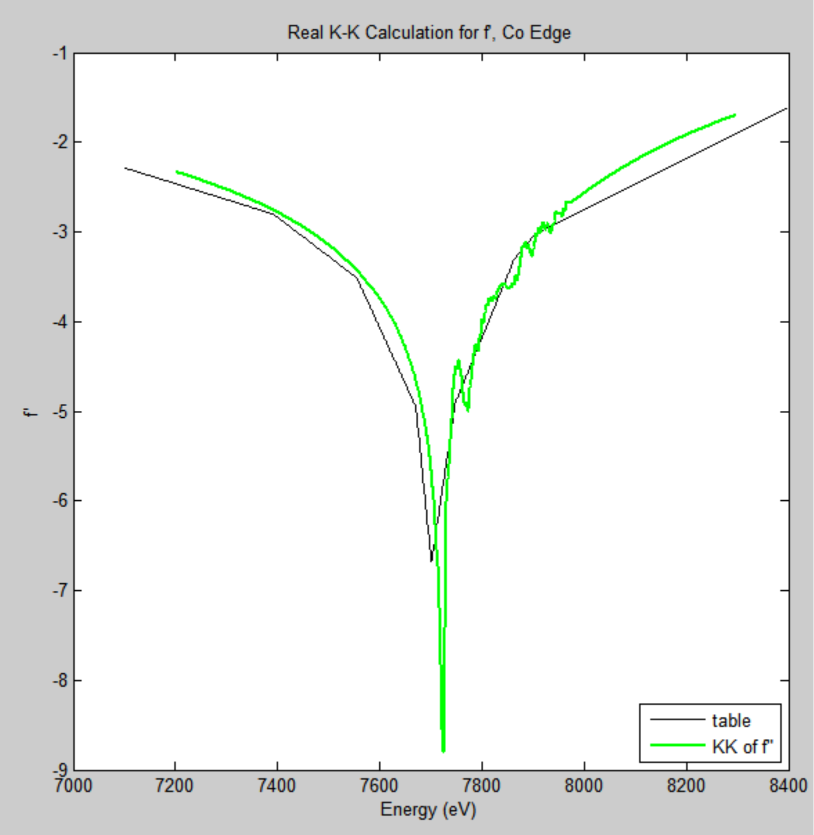
```
[ref_calc, imf_calc_all,     ref_calc_all,     energies] = kkReal(  imf,    E,    'Co', [], 1);
     ^           ^                 ^                ^                 ^      ^        ^      ^
   f’    |  f’’ over all E|   f’ over all E   |   all E        |input f’’ |inputE |Elem. |Plots on
```

and the empty bracket specifies the default energy range [E_low-100, E_high+100]

c. The plots look like:



Input f'' data, Co Edge



Real K-K Calculation for f', Co Edge

d. The outputs are arrays. I do not bother saving this information because that is easily accomplished from the output arrays.

8) Dependencies

I use a heavily modified version of Valerio Lucarini's KK transform functions, and a program that finds Z given an element name.

There is an additional function that looks up Z based on element symbol.

My program requires f' and f'' text files saved from NIST's tables. I have only saved those for the elements I used this past summer. Add elements as needed (save the maximum possible range). Instructions are in the NIST folder.