Basics of EXAFS data analysis

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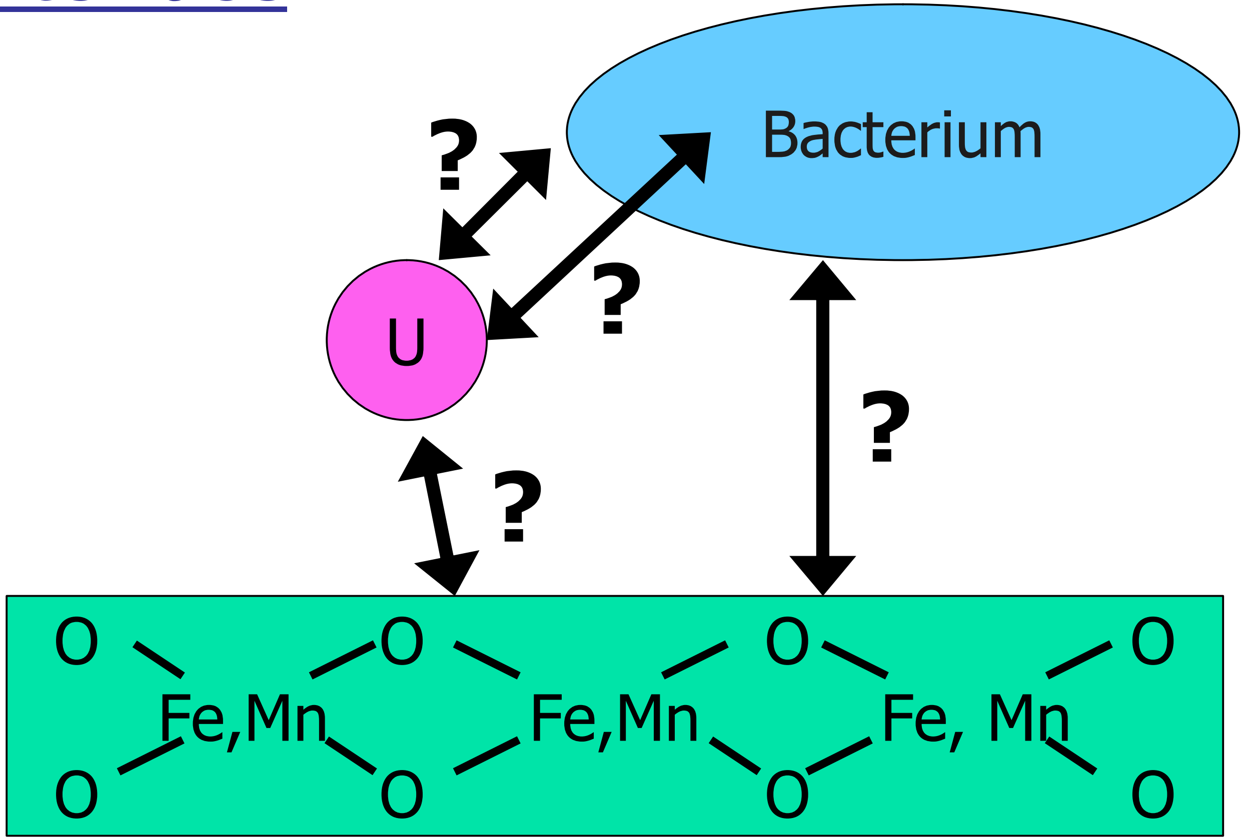
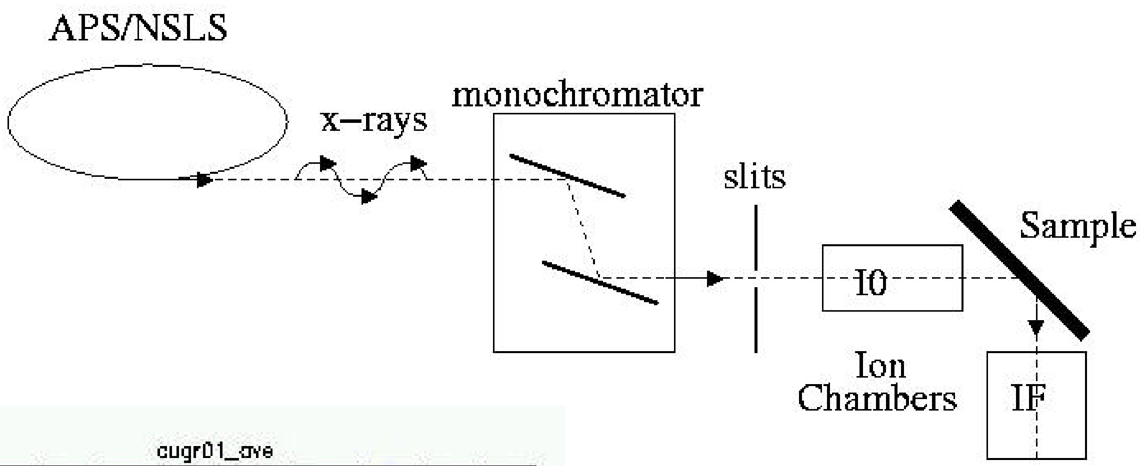
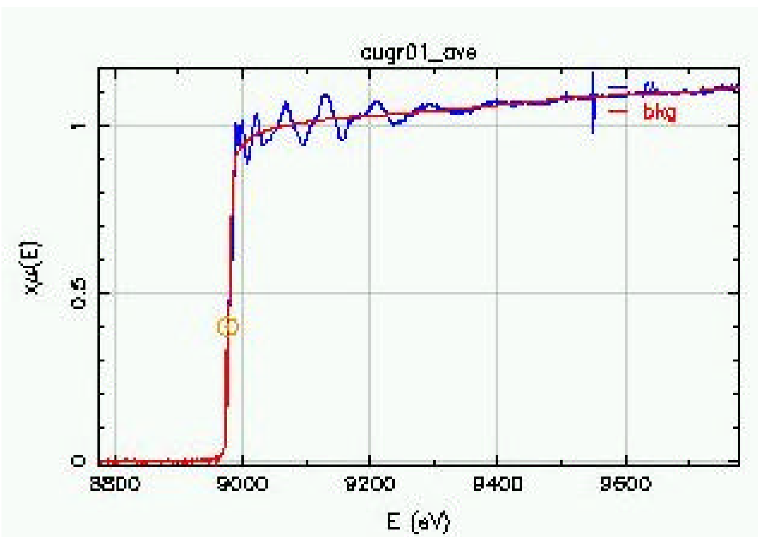
Investigation of the interactions of U Species at the Bacteria-Geosurface Interface



X-ray-Absorption Fine Structure





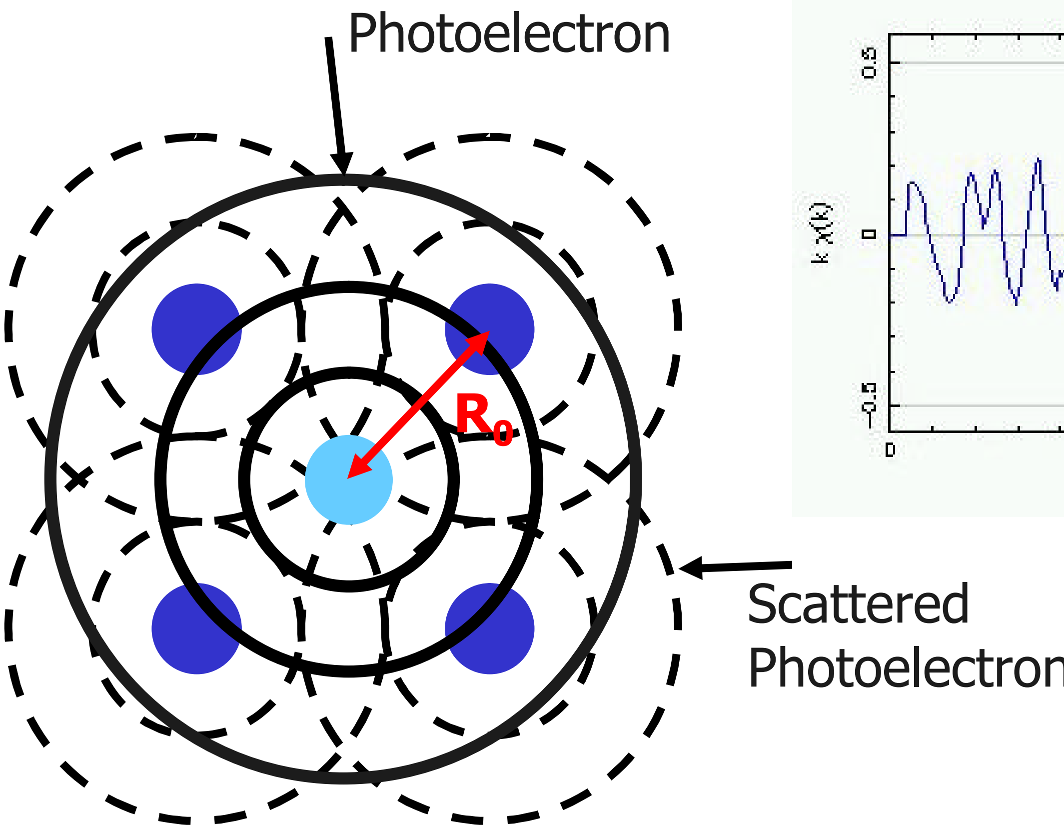
- Attenuation of x-rays

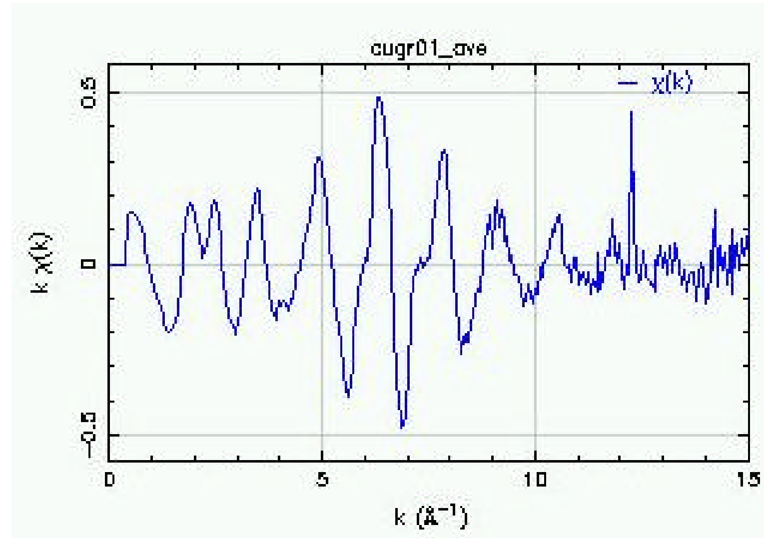
  $I_t = I_0 e^{-\mu(E) \cdot x}$

- Absorption coefficient

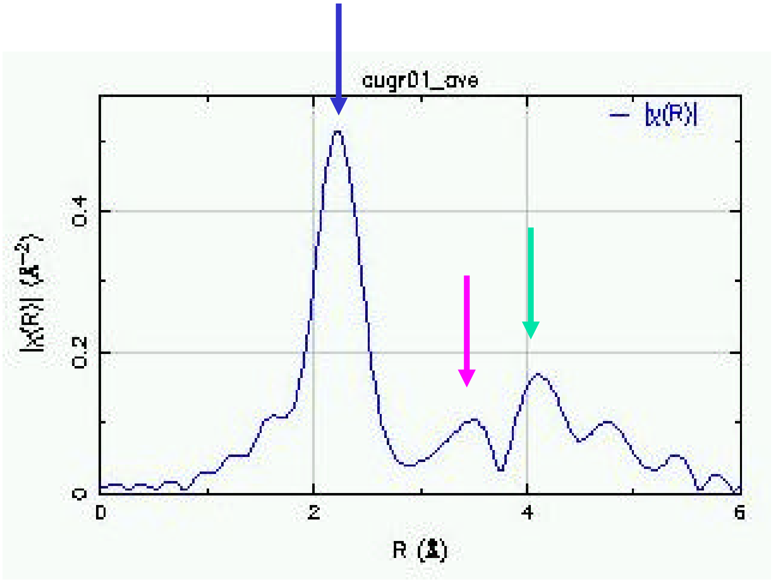
  $\mu(E) \propto I_f / I_0$

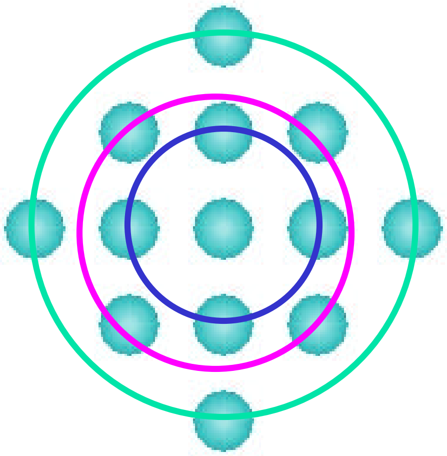
X-ray-Absorption Fine Structure





Fourier Transform of $\chi(k)$



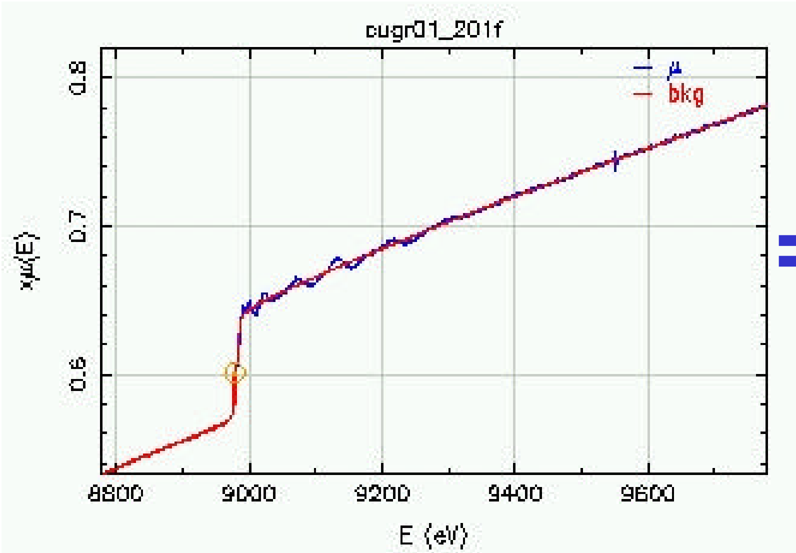


- **Similar to an atomic radial distribution function**
  - Distance
  - Number
  - Type
  - Structural disorder

Outline

- **Definition of EXAFS**
  - Energy to wave number
  - Edge Step
- **Fourier Transform (FT) of** $\chi(k)$
  - FT of sine wave is a delta function
  - FT of a discrete data set
  - Different parts of a FT and backward FT
  - FT windows and sills
  - Information content
- **Autobk method for constructing the bkg**
  - FT and background (bkg) function
  - Wavelength of bkg
  - Fit the bkg
- **EXAFS Equation**

Definition of EXAFS



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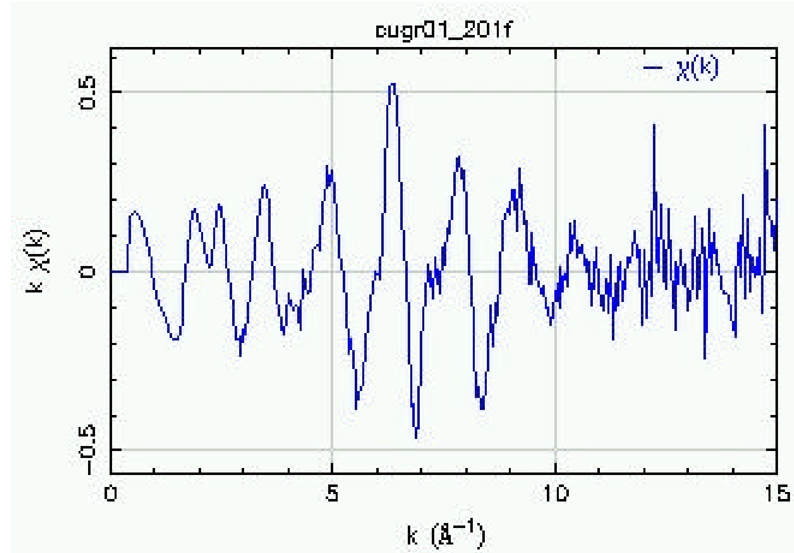


Normalized oscillatory part of absorption coefficient

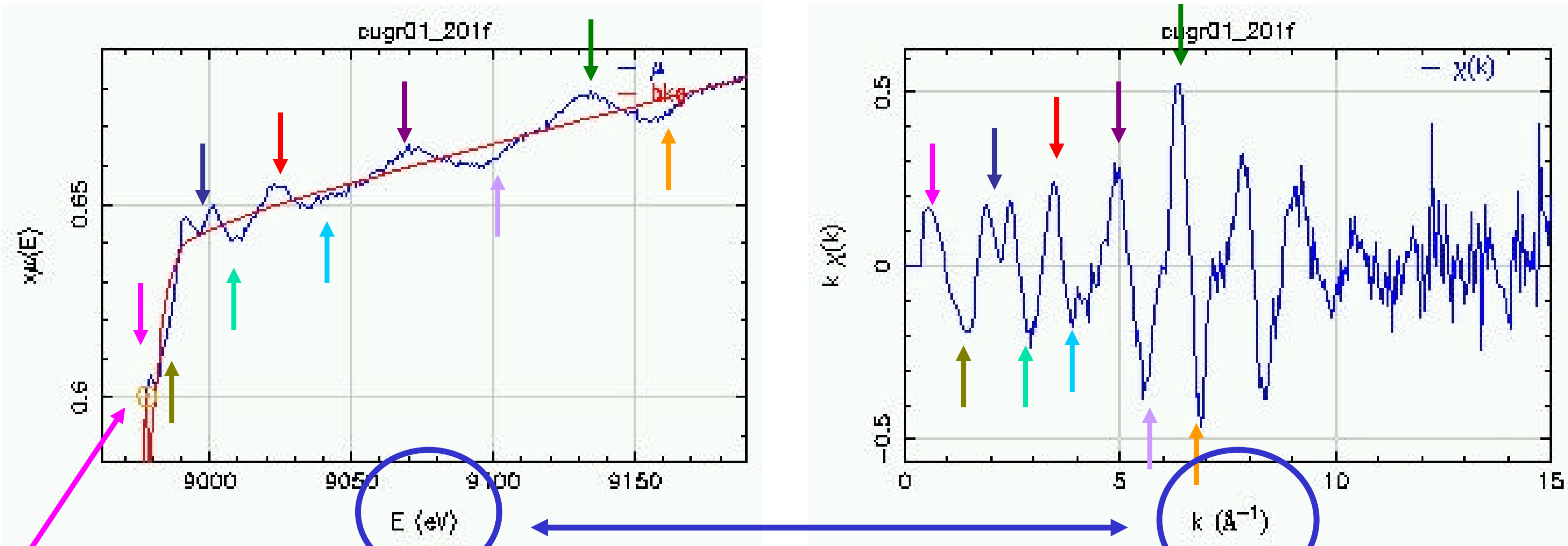
Measured Absorption coefficient

Bkg: Absorption coefficient without contribution from neighboring atoms (Calculated)

$$c(E) = \frac{m(E) - m_0(E)}{Dm(E)} \sim \frac{m(E) - m_0(E)}{Dm(E_0)}$$

Evaluated at the Edge step (E_0)

Energy to wave number



E_0 Must be somewhere on the edge

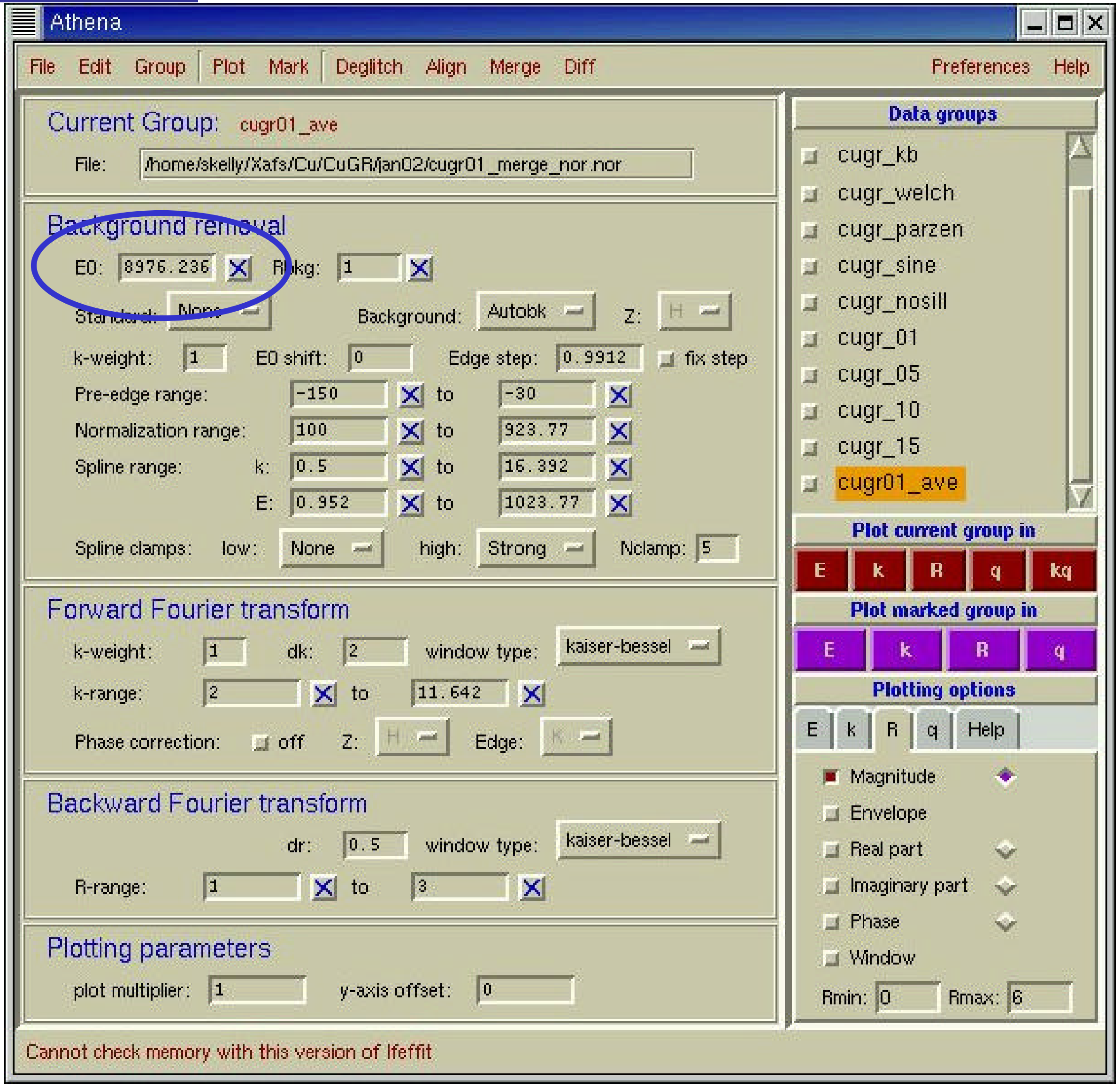
Mass of the electron

Fermi Energy

$$k^2 = \frac{2\, m_e\, (E - E_0)}{h} \sim 3.81\ \mathrm{DE}$$

Plank's constant

Athena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Background removal
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Rbkg: 1
Standard: None
Background: Autobk
Z: H
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E0 shift: 0
Edge step: 0.9912
fix step
Pre-edge range: -150 to -30
Normalization range: 100 to 923.77
Spline range: k: 0.5 to 16.392
E: 0.952 to 1023.77
Spline clamps: low: None high: Strong Nclamp: 5
Forward Fourier transform
k-weight: 1 dk: 2 window type: kaiser-bessel
k-range: 2 to 11.642
Phase correction: off Z: H Edge: K
Backward Fourier transform
dr: 0.5 window type: kaiser-bessel
R-range: 1 to 3
Plotting parameters
plot multiplier: 1 y-axis offset: 0
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cugr_parzen
cugr_sine
cugr_nosill
cugr_01
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cugr_15
cugr01_ave
Plot current group in
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Plotting options
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Magnitude
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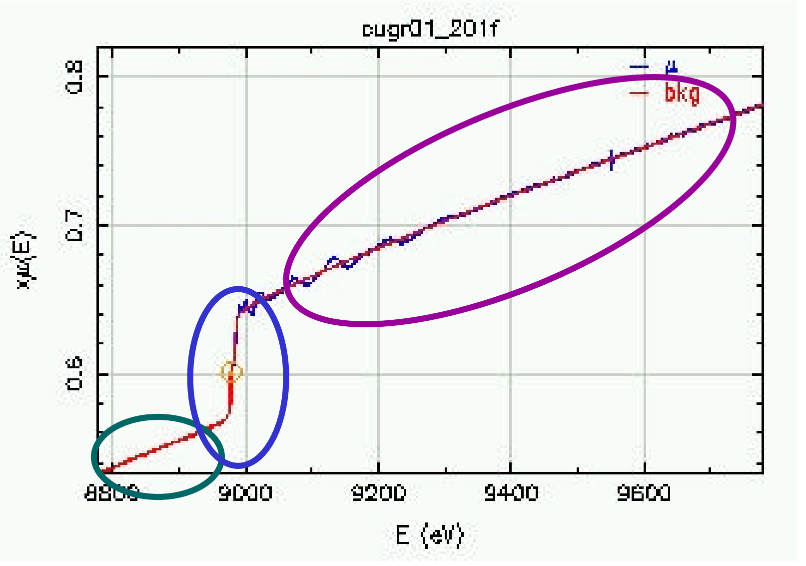
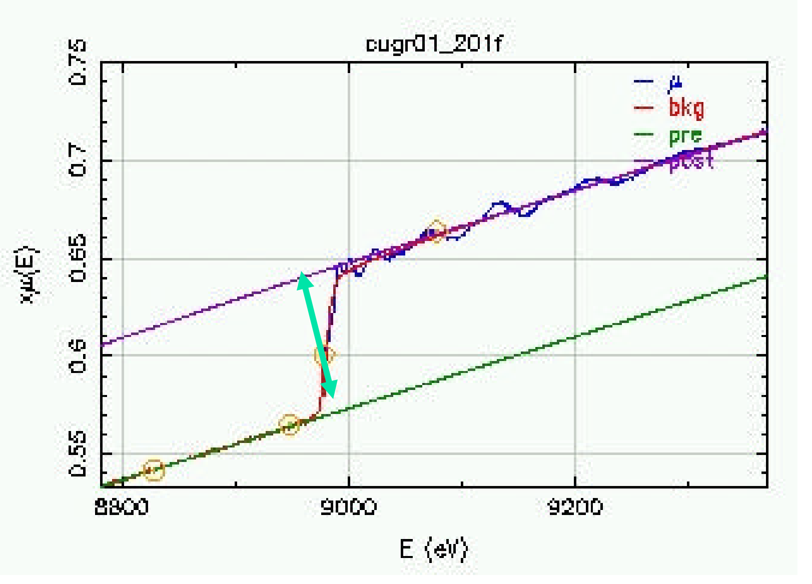
Real part
Imaginary part
Phase
Window
Rmin: 0 Rmax: 6

Absorption coefficient



- **Pre-edge region** **300 to 50 eV before the edge**
- **Edge region** **the rise in the absorption coefficient**
- **Normalization region** **50 to 1000 eV after the edge**

Edge step



- **Pre-edge line** 200 to 50 eV before the edge
- **Normalization line** 100 to 1000 eV after the edge
- **Edge step** the change in the absorption coefficient at the edge
  - Evaluated by taking the difference of the pre-edge and normalization lines at E_0

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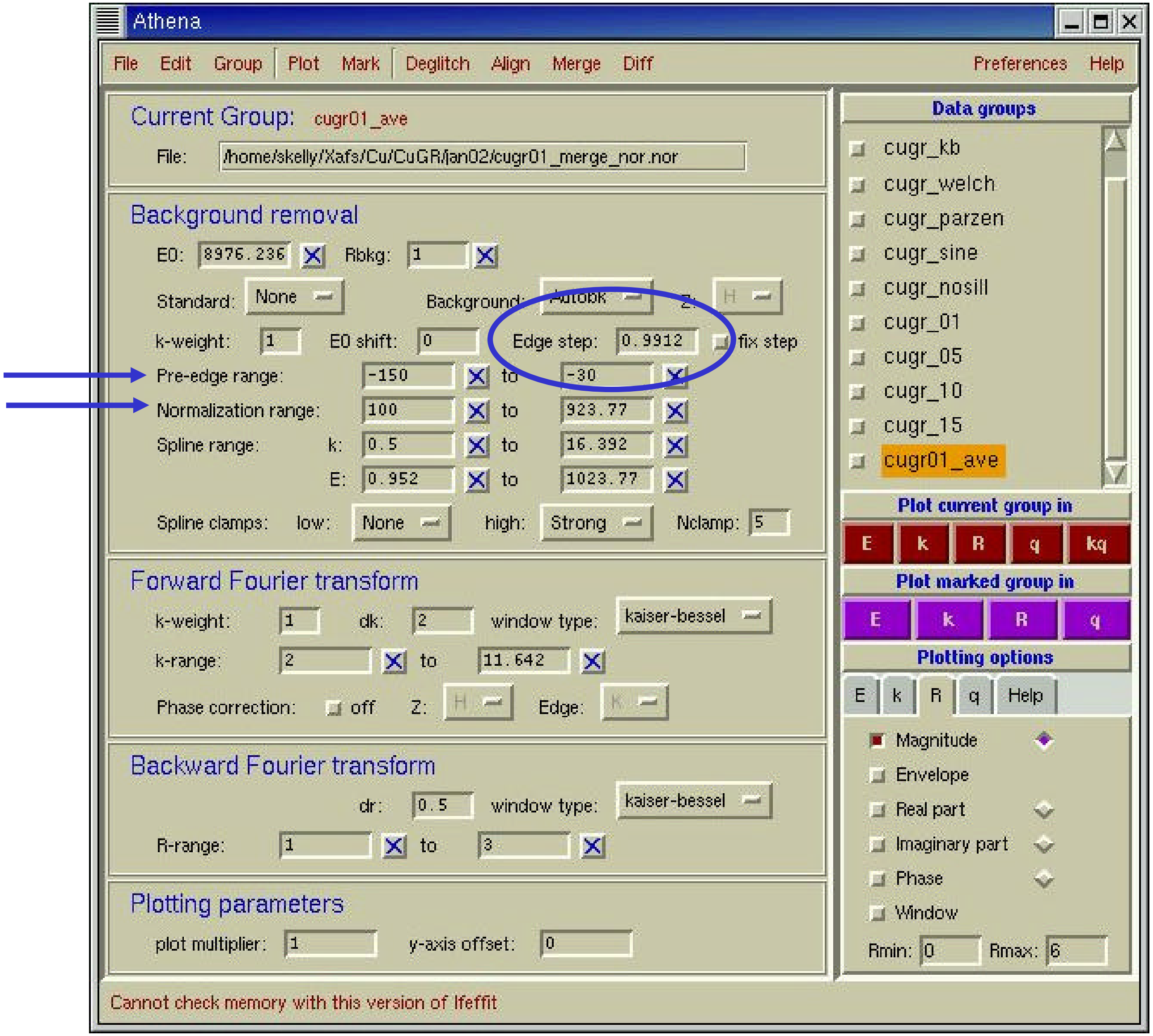
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Plot marked group in
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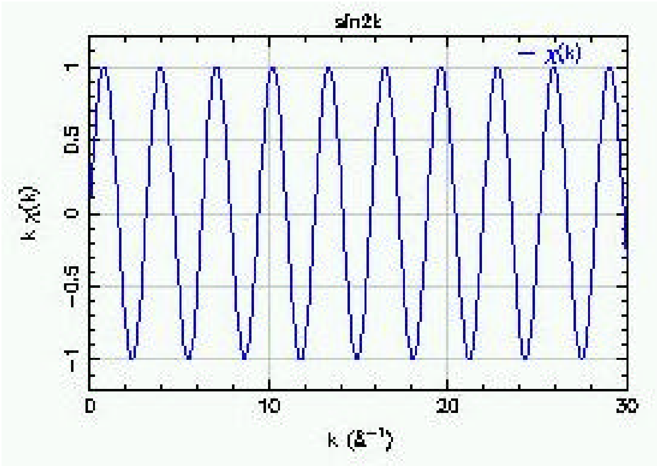
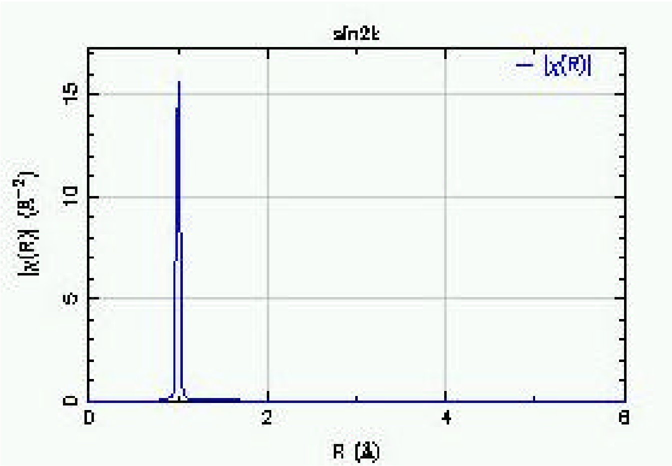
Real part
Imaginary part
Phase
Window
Rmin: 0 Rmax: 6

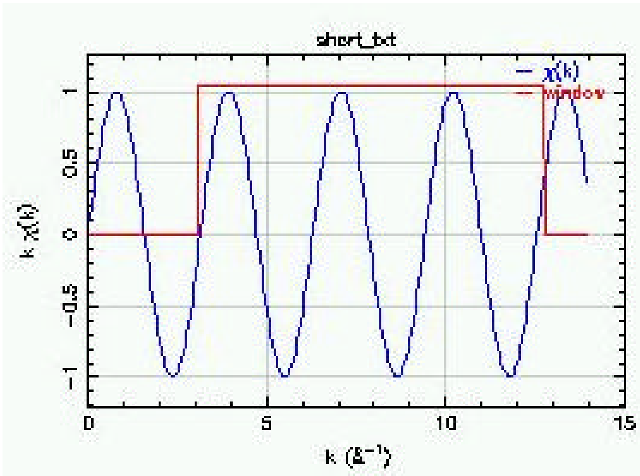
Fourier Transform

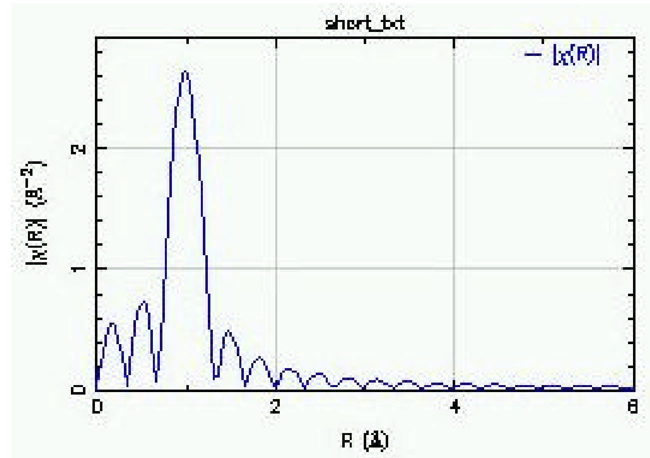




FT of infinite sine wave is a delta function

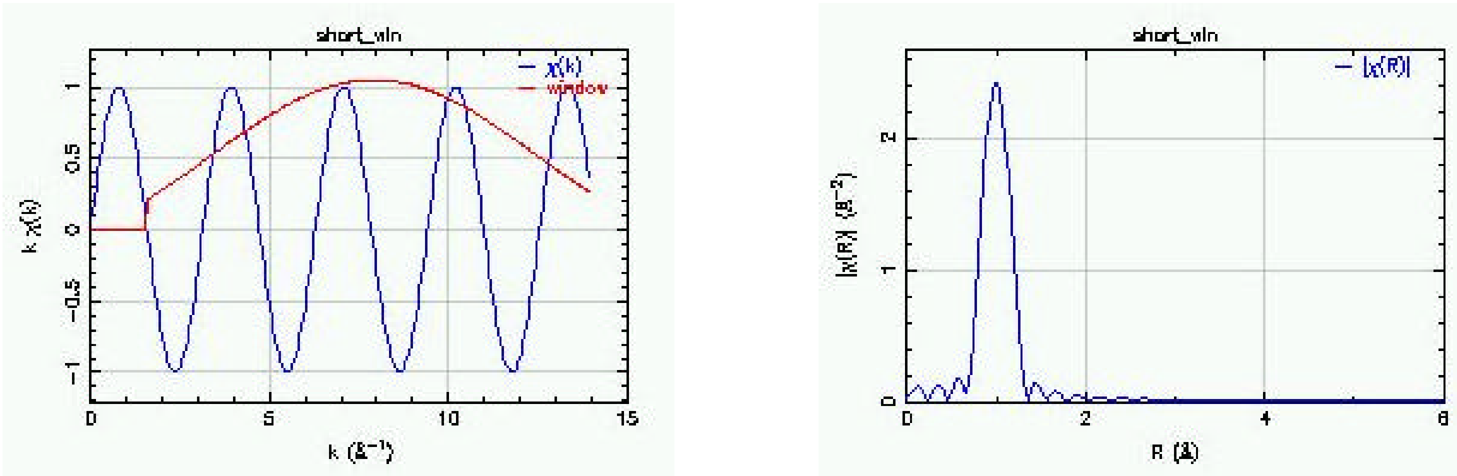
Fourier Transform





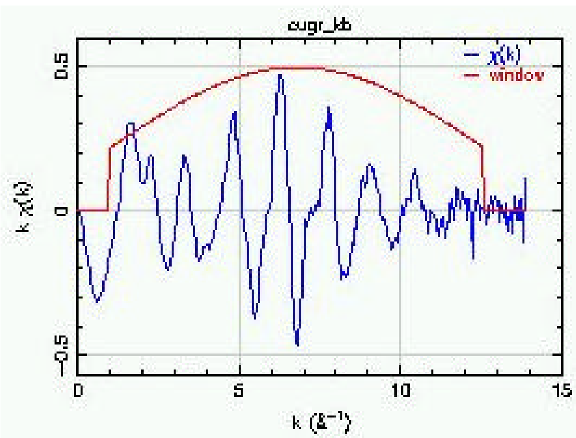
- **FT of discrete sine wave is a distorted peak**
- **Localized features in k-space become unlocalized in R-space**

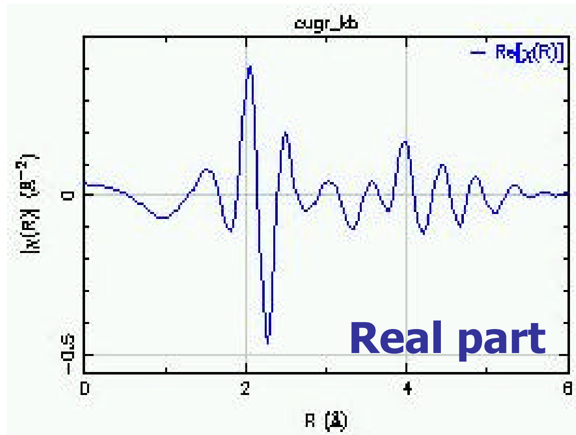
Fourier Transform

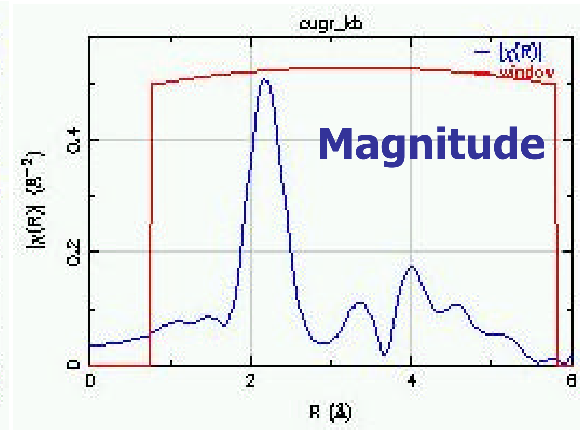


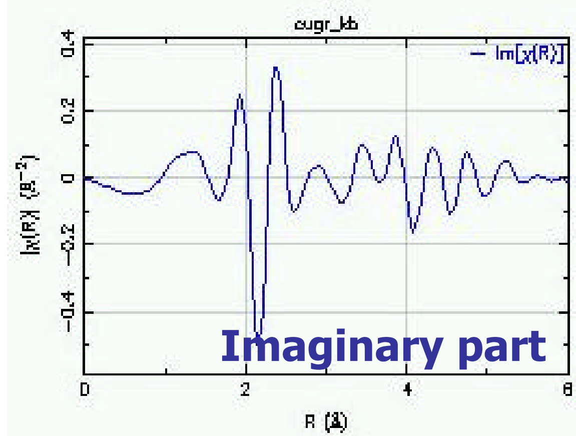
- **Multiplying the sine wave by a window that gradually increases the amplitude of the sine wave smoothes the FT of discrete sine wave is a distorted peak**

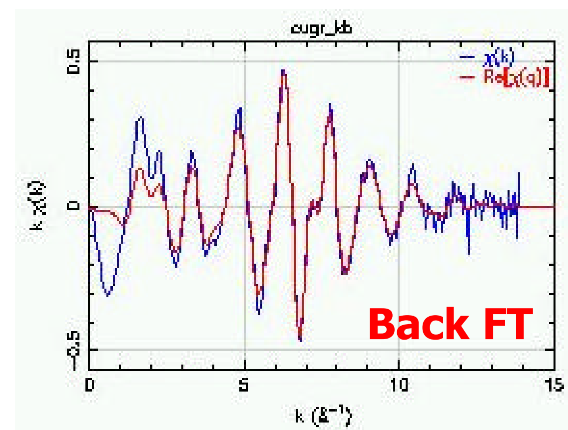
Fourier Transform parts



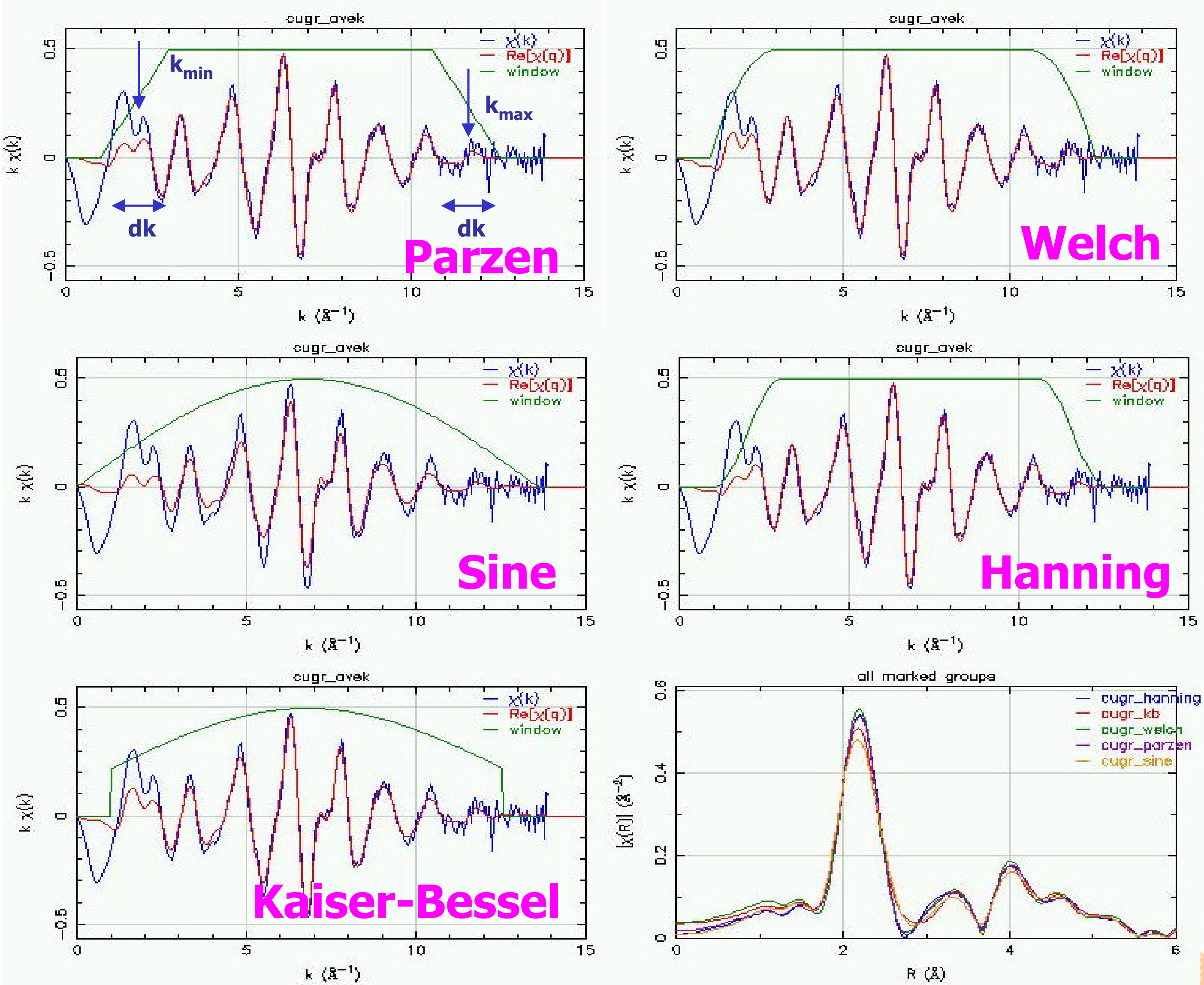




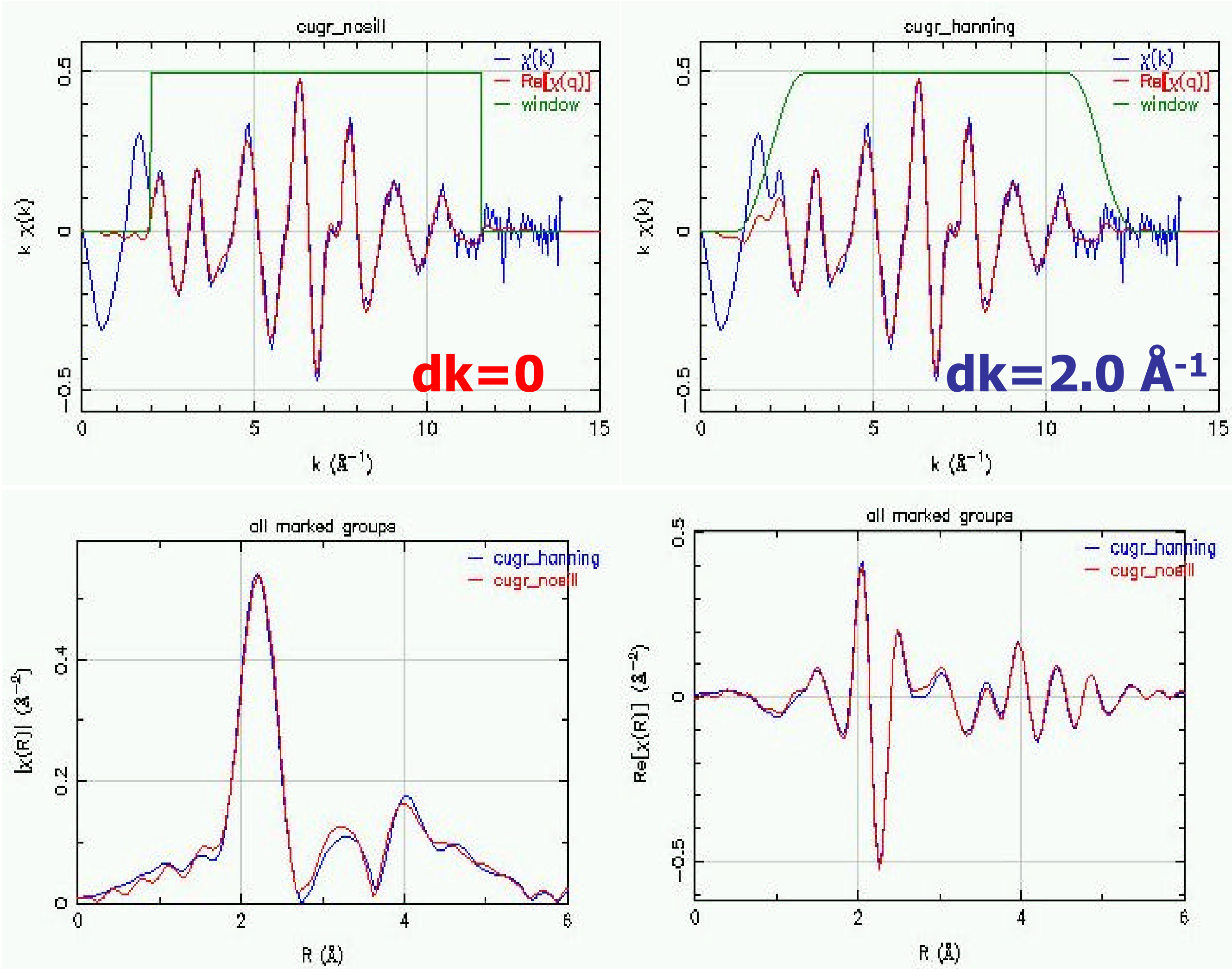




Fourier Transform Windows



Fourier Transform window sill



- **A small sill can distort FT**

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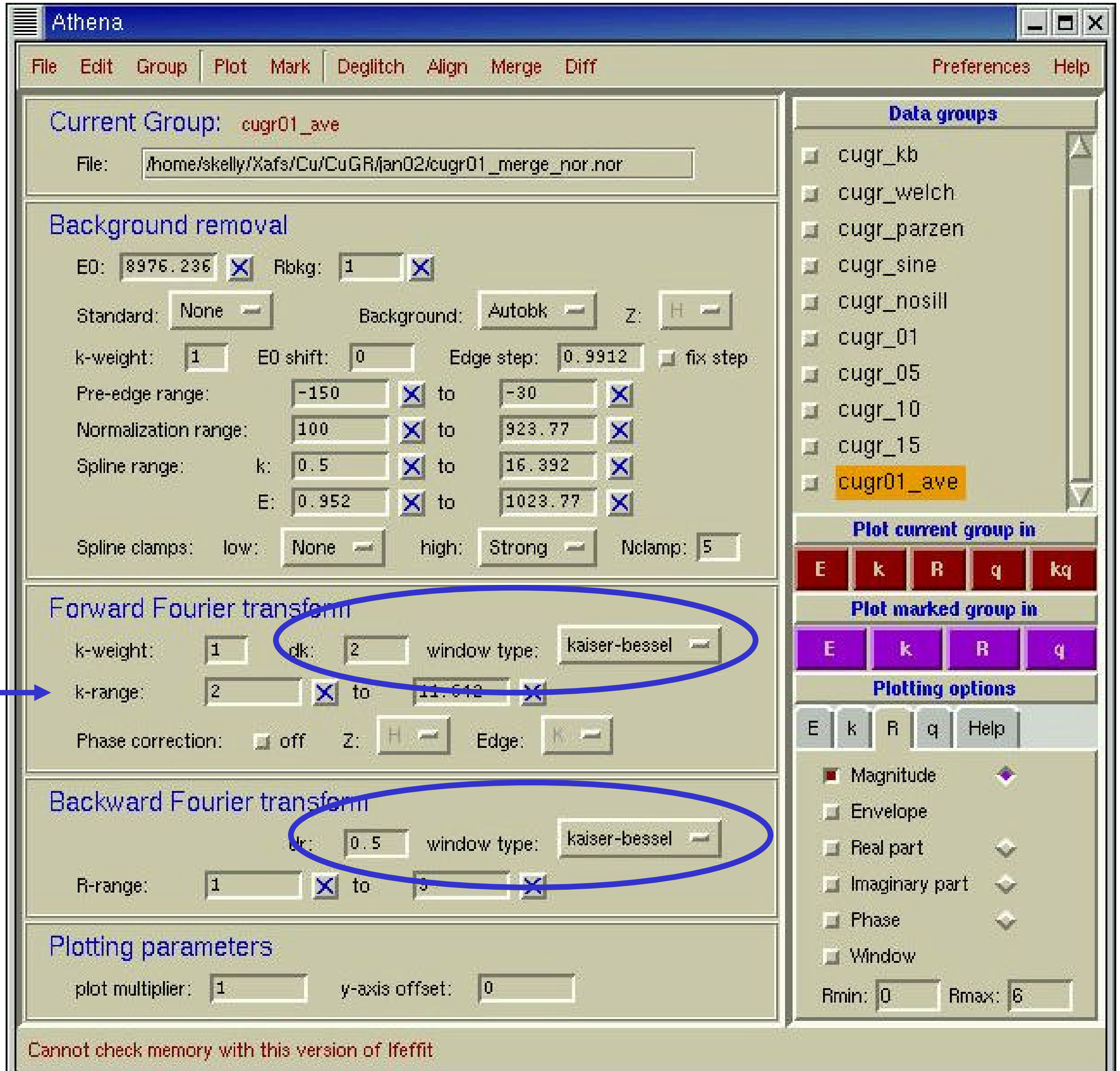
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Background removal
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Standard: None Background: Autobk Z: H
k-weight: 1 E0 shift: 0 Edge step: 0.9912 fix step
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k-range: 2 to
Phase correction: off Z: H Edge: K
Backward Fourier transform
dr: 0.5 window type: kaiser-bessel
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Plotting parameters
plot multiplier: 1 y-axis offset: 0
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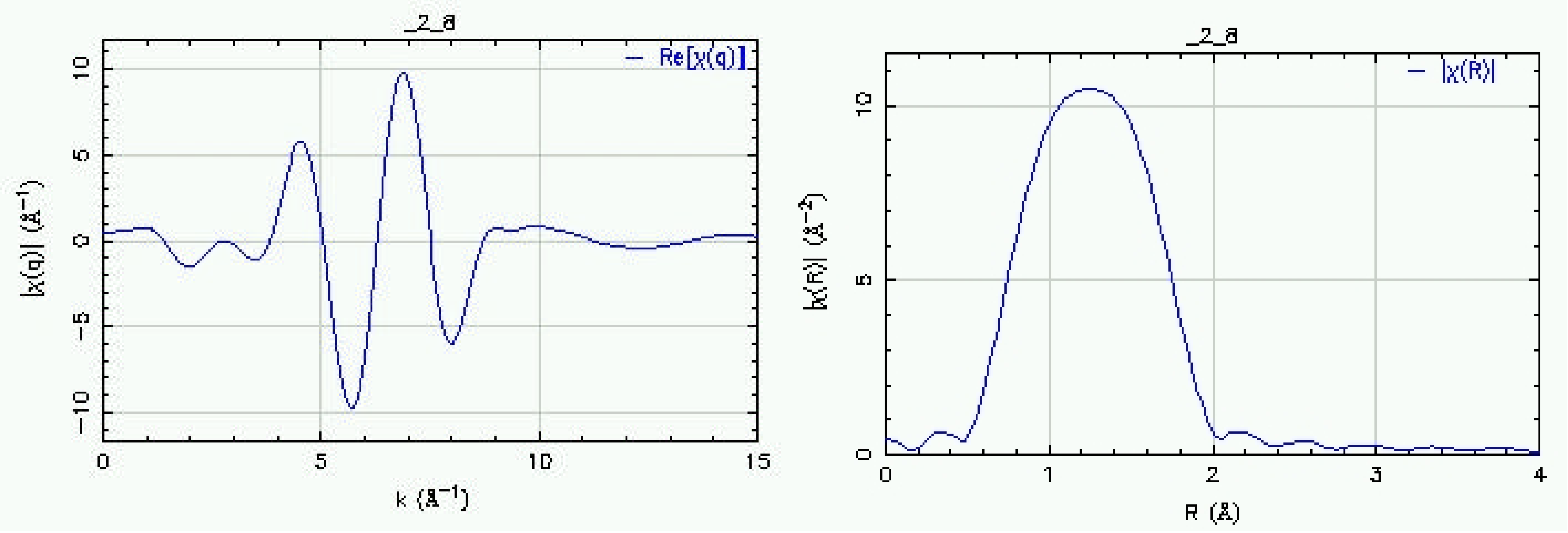
Plotting options
E k R q Help
Magnitude
Envelope
Real part
Imaginary part
Phase
Window
Rmin: 0 Rmax: 6

Information content

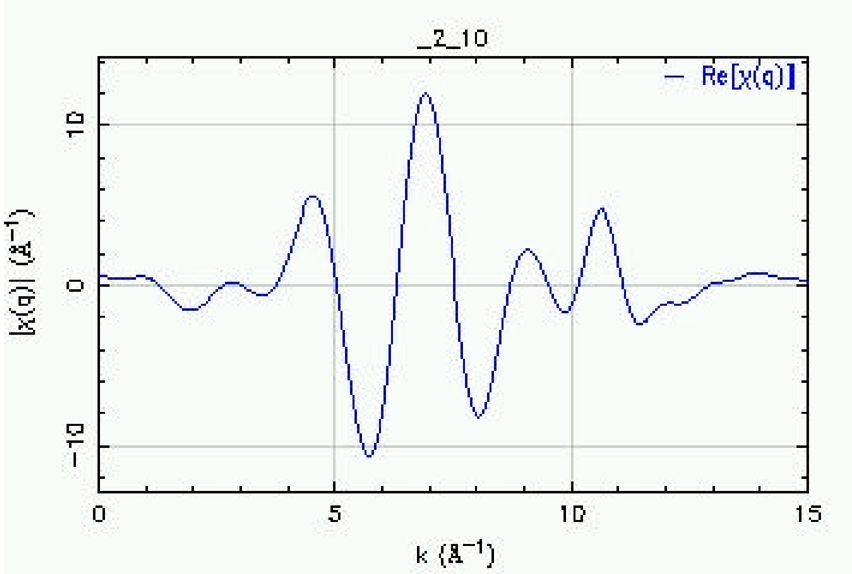
FT k-range = 2-8 Å^{-1}

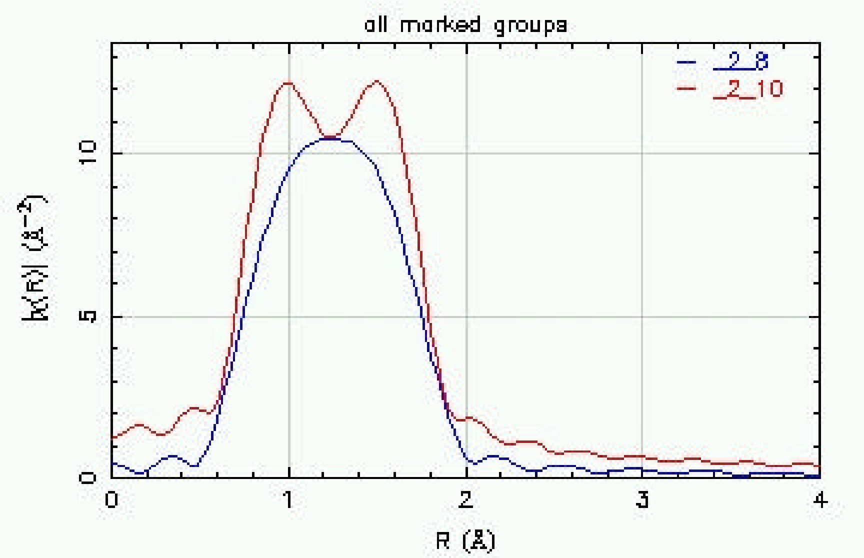


- **The amount of information in the data depends on the k-range and the R-range**

Information content

FT k-range = 2-10 Å^{-1}

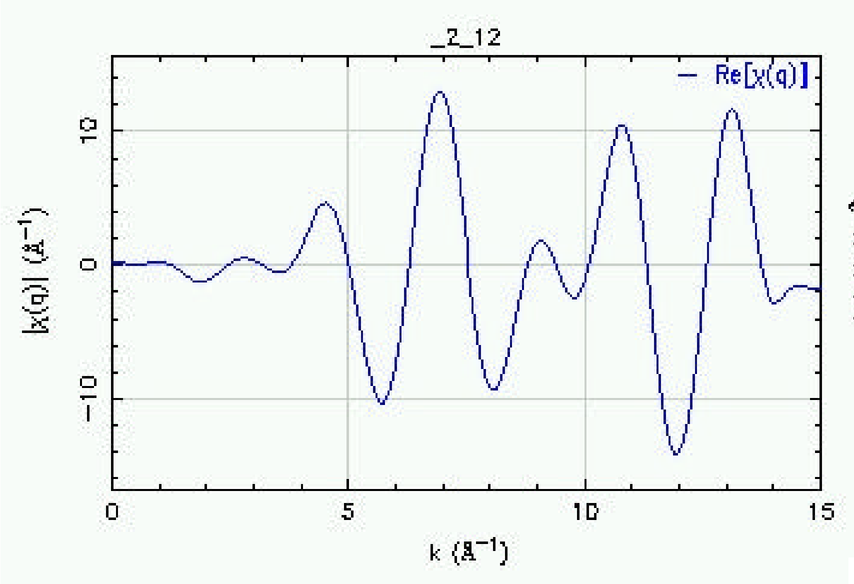


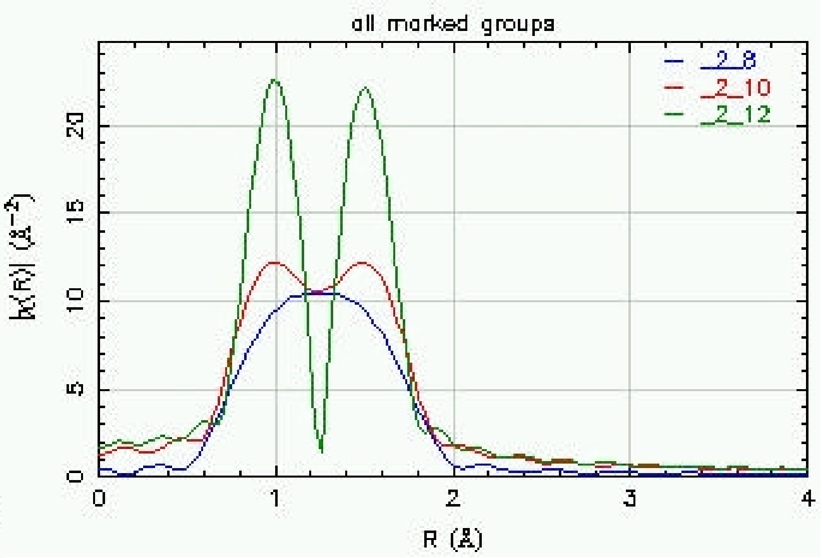


- **The amount of information in the data depends on the k-range and the R-range**

Information content

FT k-range = 2-12 Å^{-1}

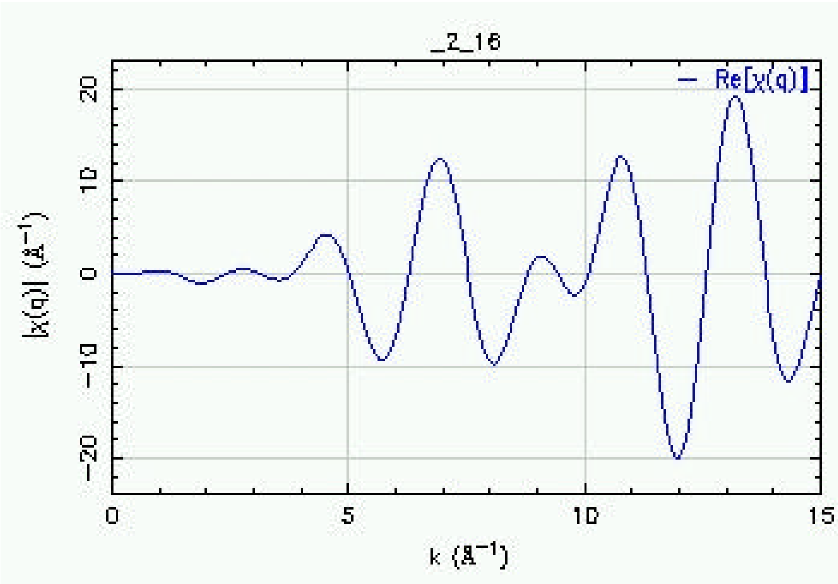


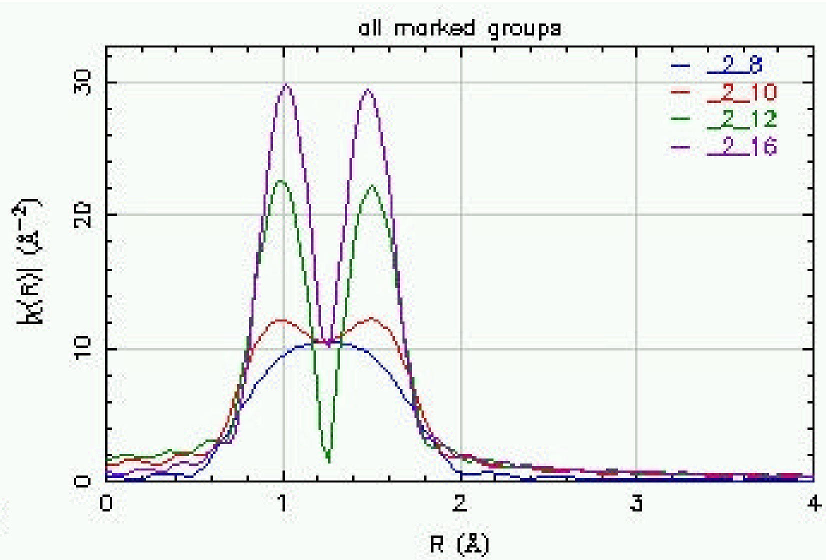


- **The amount of information in the data depends on the k-range and the R-range**

Information content

FT k-range = 2-16 Å^{-1}

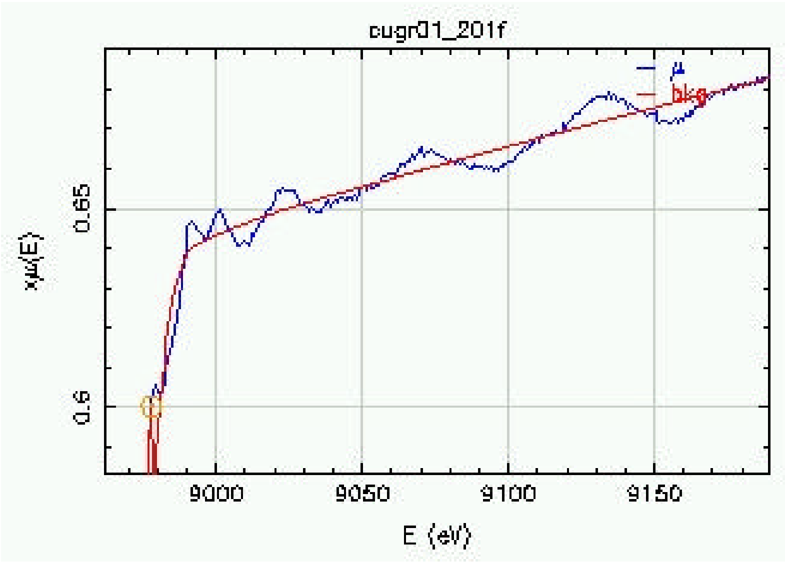


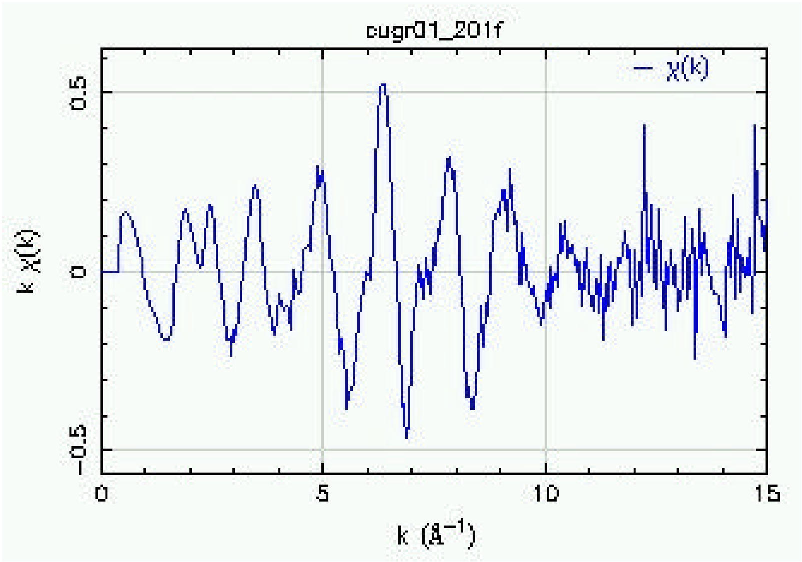


$$\chi(k) = \sin(2k) + \sin(3k)$$

Number of independent points $\sim \dfrac{2\,\Delta R\,\Delta k}{\pi}$

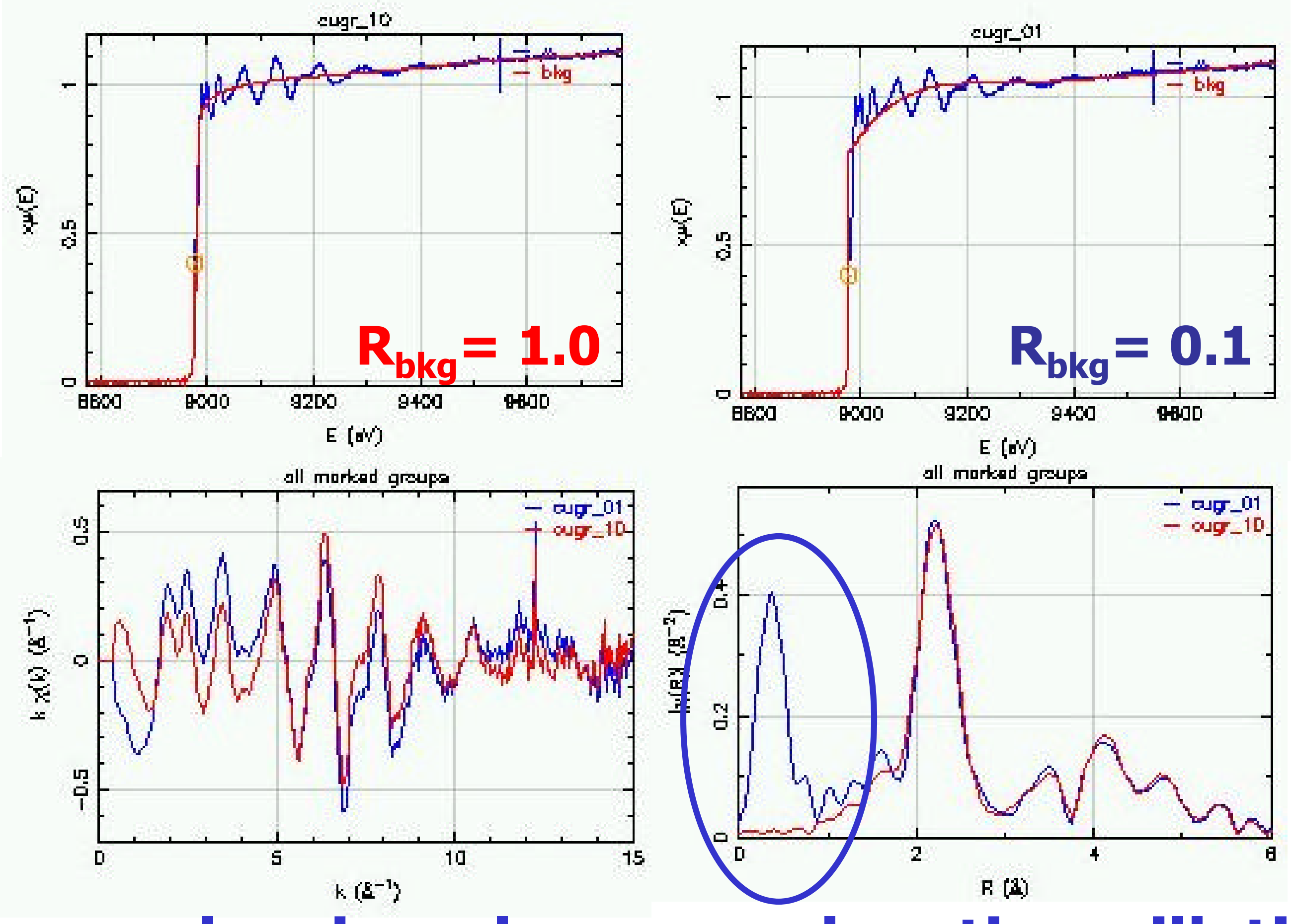
Background function overview





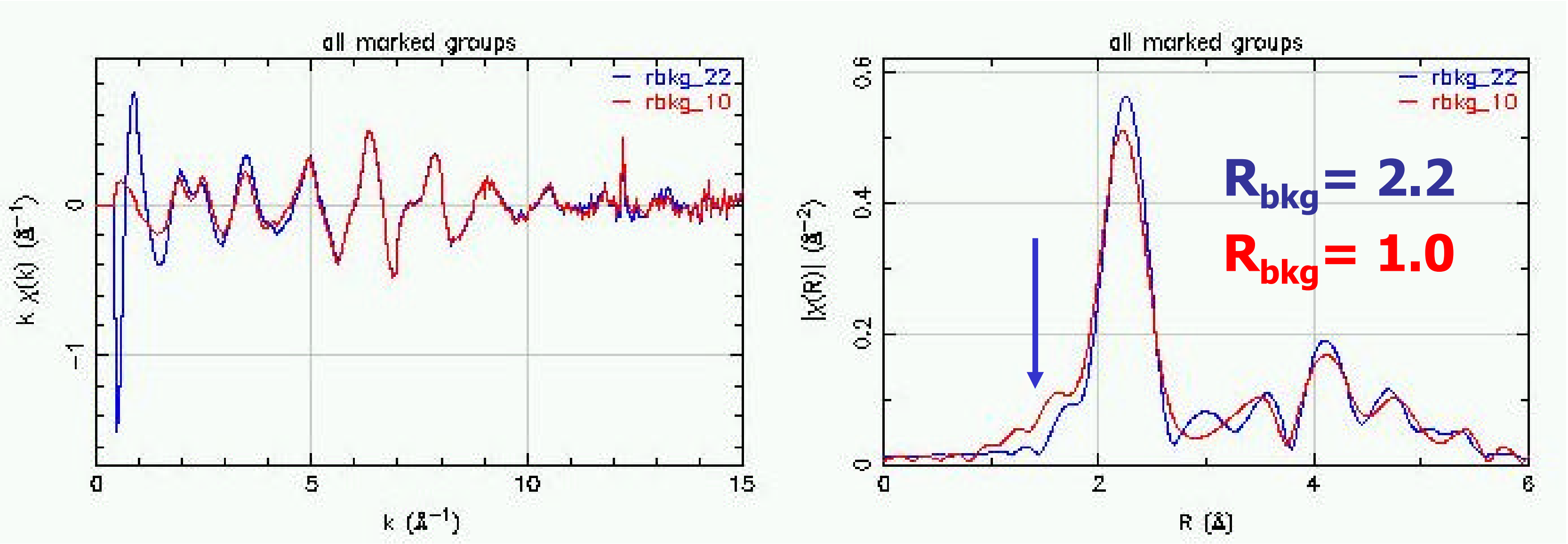
- **A good background function removes long wavelength oscillations from c(k).**
- **Long wavelength oscillations in c(k) will appear as peaks in FT at less than half the R-value for the first peak.**
- **Constrain background so that it cannot contain wavelengths that are part of the data.**

FT and Background function



- **An example where long wavelength oscillations appear as (false) peak in the FT**

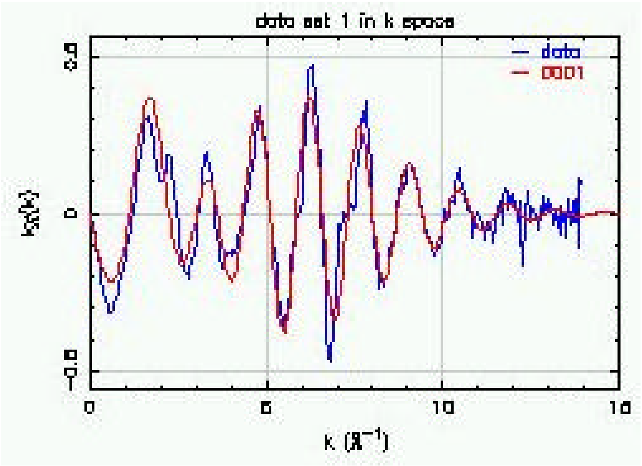
FT and Background function



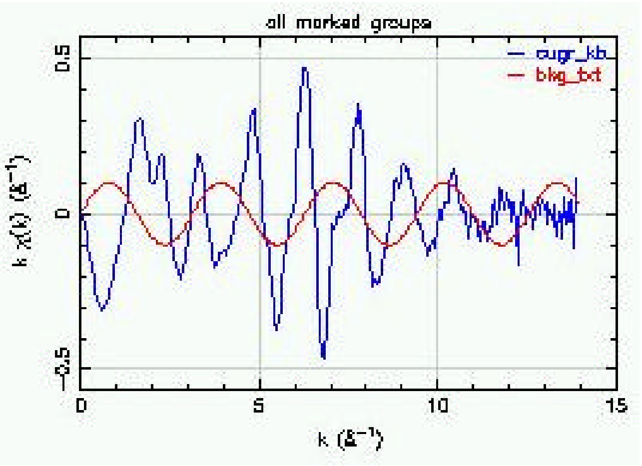
- **An example where background distorts the first shell peak.**
- **R_{bkg} should be about half the R value for the first peak.**

Frequency of Background function

Data contains this and shorter wavelengths

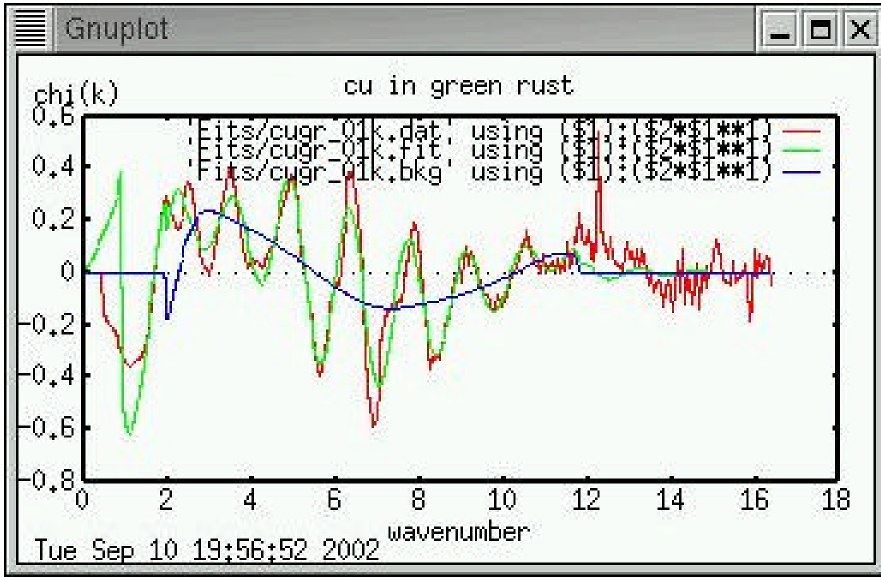


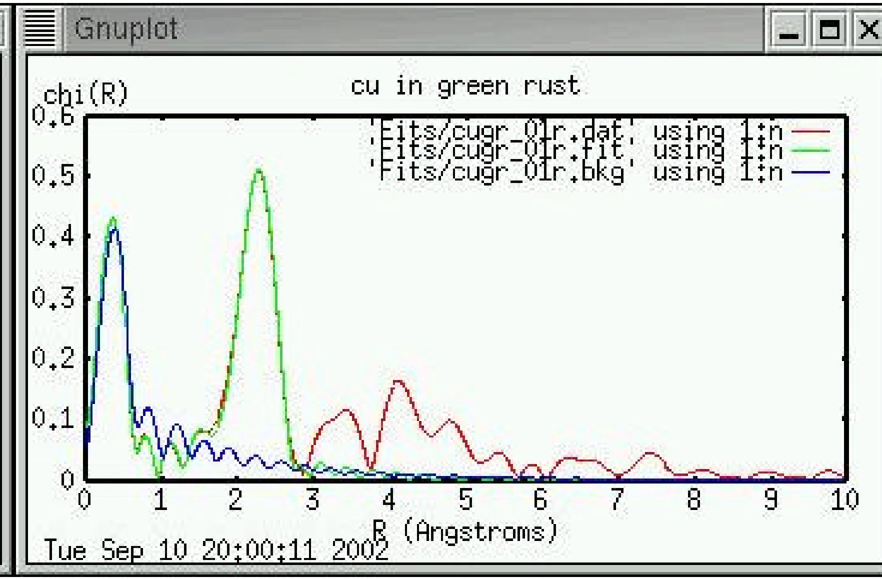
Bkg contains this and longer wavelengths



- **Constrain background so that it cannot contain wavelengths that are part of the data.**
  - Use information theory, number of knots = $2\ R_{bkg}\ \Delta k\ /\ \pi$
  - 9 knots in bkg using R_{bkg}=1.0 and Δk = 14.0
- **Background may contain only longer wavelengths. Therefore knots are not constrained.**

Fit the background function





11 knots in bkg = $\frac{2 R_{bkg} \Delta k}{\pi}$ using R_{bkg} = 1.8 and Δk = 9.7

- **Knots are not fixed**
- **shortest wave length constrained by R_{bkg}.**
- **Not yet implemented in Artemis?**

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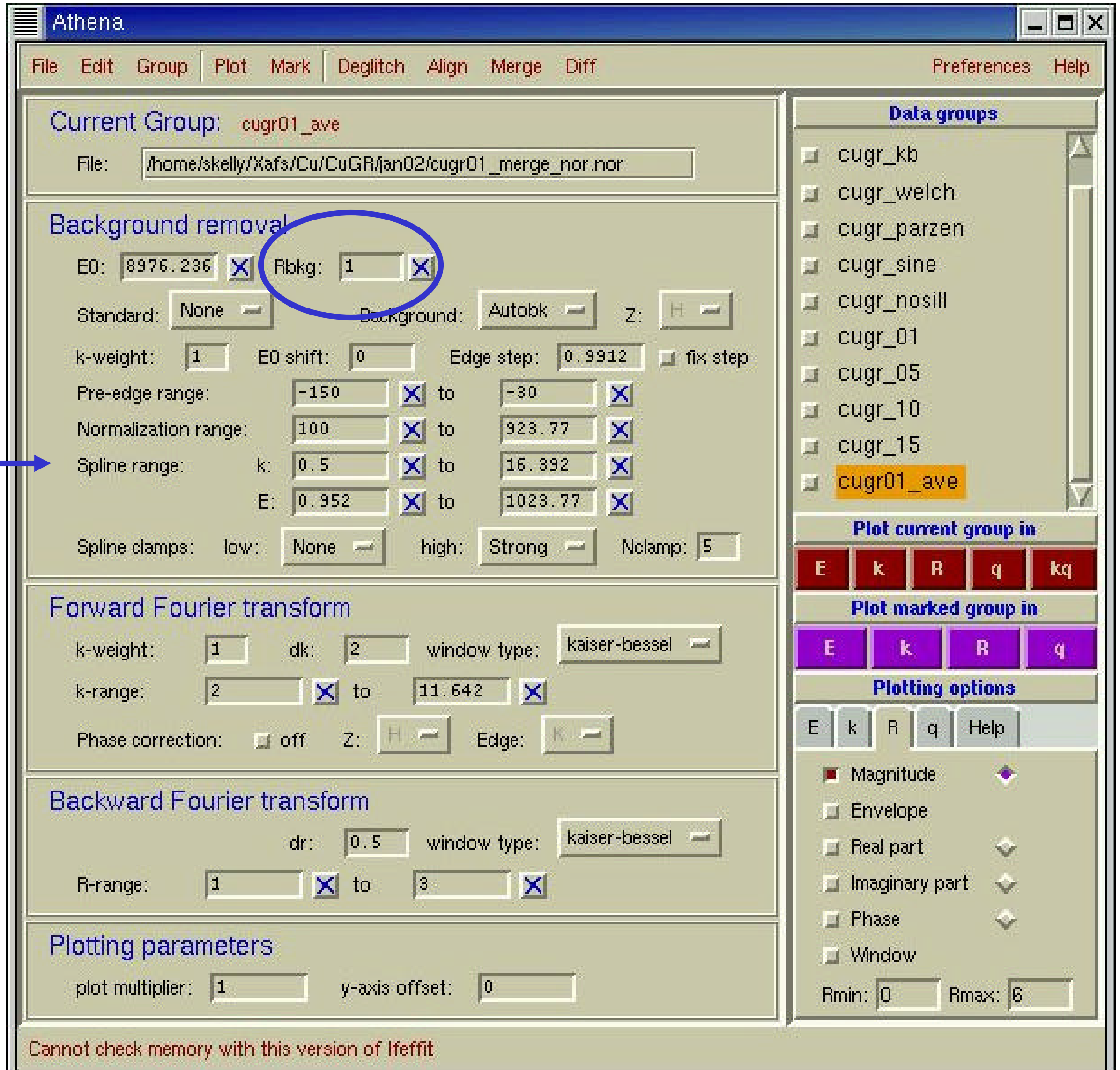

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Plotting options
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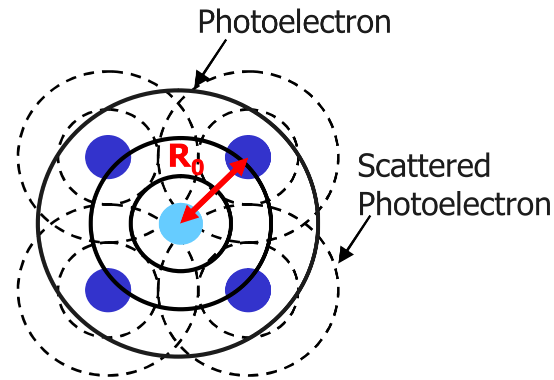
Rmax: 6

The EXAFS Equation



$$\chi(k) = \Sigma_i\ \chi_i(k)$$

with

$$\chi_i(k) = \text{Im}\left(\frac{(N_i S_0^2) F_i(k)}{kR_i^2}\ \exp(i(2kR_i + \varphi_i(k))\ \exp(-2\sigma_i^2 k^2)\ \exp(-2R_i/\lambda(k))\right)$$

$$R_i = R_0 + \Delta R$$

$$k^2 = 2\ m_e(E-E_0)/\ h$$

Theoretically calculated values

- $F_i(k)$ effective scattering amplitude
- $\varphi_i(k)$ effective scattering phase shift
- $\lambda(k)$ mean free path
- R_0 initial path length

Parameters often determined from a fit to data

- N_i degeneracy of path
- S_0^2 passive electron reduction factor
- σ_i^2 mean squared displacement
- E_0 energy shift
- ΔR change in half-path length