X-ray Absorption Fine-Structure Spectroscopy: Theory

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Fundamentals of X-ray Absorption Fine-Structure

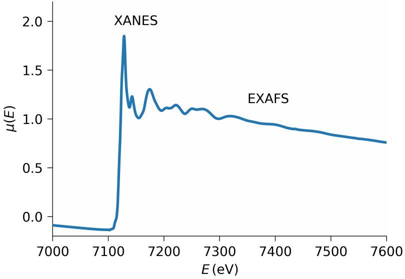
Virtual XAFS School at Illinois Institute of Technology and Advanced Photon Source

X-ray Absorption Spectroscopy: XAS, XAFS, EXAFS and XANES.

X-ray Absorption Spectroscopy (XAS) is the modulation of the X-ray absorption coefficient at energies at and above an X-ray absorption edge.

XAFS	X-ray Absorption Fine-Structure Spectroscopy (= XAS)
XANES	X-ray Absorption Near-Edge Spectroscopy
EXAFS	Extended X-ray Absorption Fine-Structure

These contain information about an element's chemical state (XANES) and local atomic environment (EXAFS).



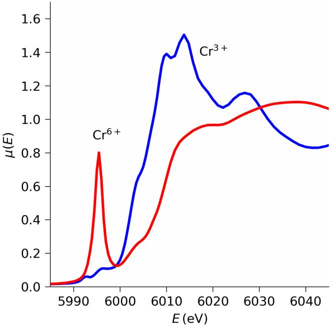
Fe K-edge XAFS for FeO

Main XAS Characteristics:

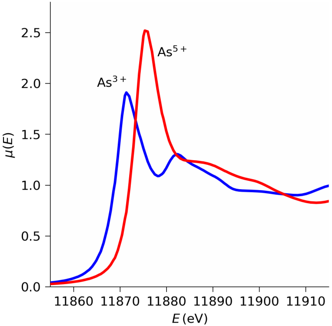
- local atomic coordination
- valence, oxidation state
- applies to any element ($Z > 2$) .
- works at low concentrations (ppm, μM)
- minimal sample requirements.
- independent of crystal structure, isotope.

XANES: X-ray Absorption Near-Edge Spectroscopy

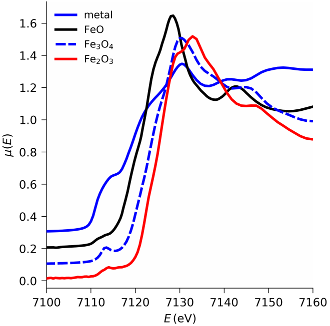
Within ∼100eV of the absorption edge, the X-ray Absorption Spectra is highly sensitive to the chemical state and formal valence of absorbing element:



Cr^{3+} and Cr^{6+}



As^{3+} and As^{5+}



Fe metal and oxides.

The oxidation state and local atomic coordination environment strongly affect the lowest unfilled electronic levels of an absorbing atom.

what are the unoccupied electronic states that the photo-electron can fill?

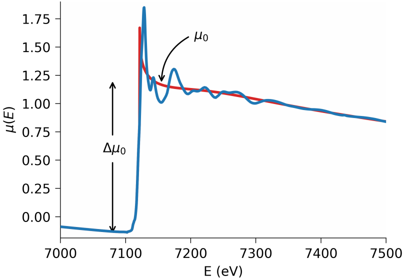
EXAFS: Extended X-ray Absorption Fine Structure

Far above the edge, the oscillations in $\mu(E)$ are sensitive to the distances and types of atoms neighboring the absorbing atom.

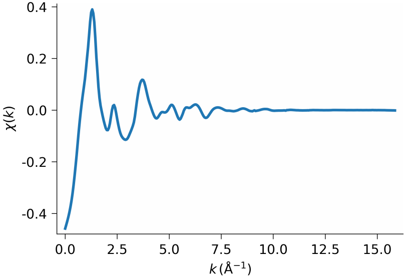
We define the EXAFS χ as the oscillations in $\mu(E)$:

$$\mu(E) = \mu_0(E)[1 + \chi(E)] \qquad \chi(E) = \frac{\mu(E) - \mu_0(E)}{\Delta\mu_0(E_0)}$$

We subtract off a smooth *"bare atom" background* $\mu_0(E)$, and divide by the *"edge step"* $\Delta\mu_0(E_0)$ to get χ, the EXAFS oscillations:



$\mu(E)$ and $\mu_0(E)$ for FeO



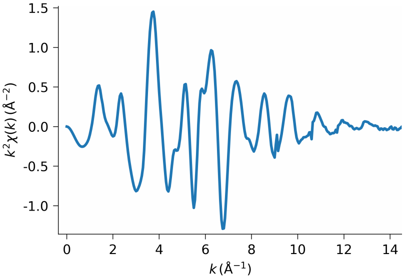
$\chi(E)$ for FeO

EXAFS: $\chi(k)$ and XAFS Fourier Transforms

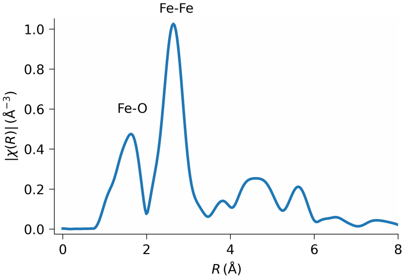
EXAFS is an *interference effect*, using the wave-nature of the photo-electron. We express the XAFS in terms of *photo-electron wavenumber*, k:

$$k = \sqrt{\frac{2m(E - E_0)}{\hbar^2}}$$

We'll also then use Fourier Transforms to convert from k to R.



$k^2\chi(k)$ for FeO



Fourier Transform $|\chi(R)|$ for FeO.
Similar to a Pair Distribution Function.

The EXAFS Equation

To model the EXAFS, we use the *EXAFS Equation*:

$$\chi(k) = \sum_j \frac{N_j f_j(k) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{k{R_j}^2} \sin[2kR_j + \delta_j(k)]$$

where $f(k)$ and $\delta(k)$ are *photo-electron scattering properties* of the neighboring atom [and $\lambda(k)$ is the photo-electron mean-free-path].

If we know these properties, we can determine:

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N	coordination number of neighboring atom.
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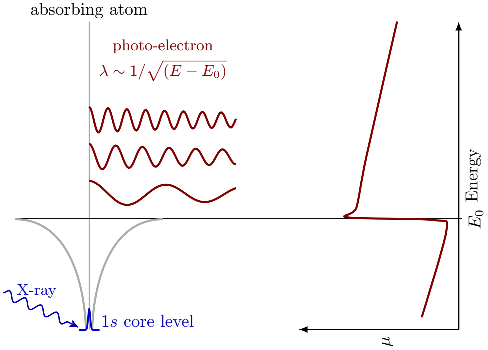
R	distance to neighboring atom.
N	coordination number of neighboring atom.
σ^2	mean-square disorder of neighbor distance.

$f(k)$ and $\delta(k)$ depend on atomic number Z of the scattering atom, so we can also determine the species of the neighboring atom.

Development of the EXAFS Equation

X-ray Absorption by a Free Atom

An atom absorbs an X-ray (energy E), destroying a core electron (energy E_0) and creating a photo-electron (energy $E - E_0$). The core hole is eventually filled, and a fluorescence X-ray or Auger electron is ejected from the atom.



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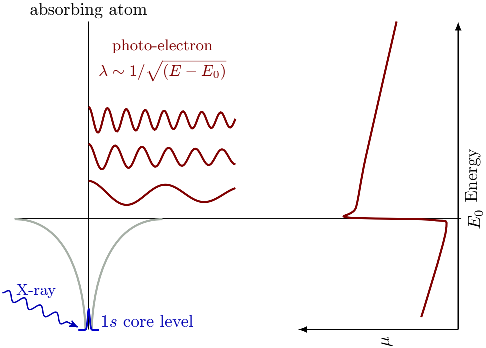

X-ray absorption needs an available state for the photo-electron to go into:

No available state:
No absorption

Once the X-ray energy is large enough to promote a core-level to the continuum, there is a sharp increase in absorption.

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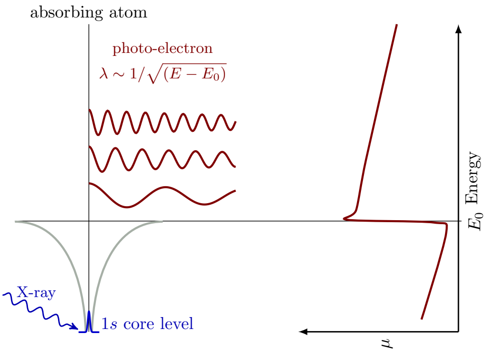

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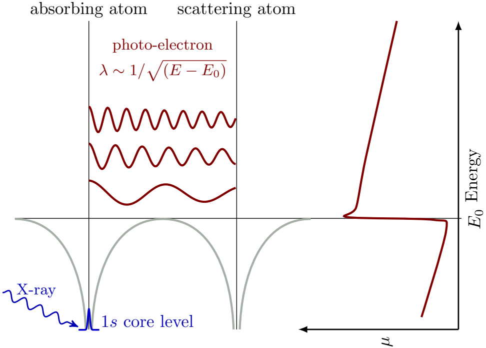
$\mu(E)$ has a sharp step at the core-level binding energy, and is a smooth function of energy above this absorption edge.

X-ray Absorption with Photo-Electron Scattering

With another atom nearby, the ejected photo-electron can *scatter* from a neighboring atom. The amplitude of the photo-electron scattered back to *the absorbing atom* will cause oscillations in $\mu(E)$.



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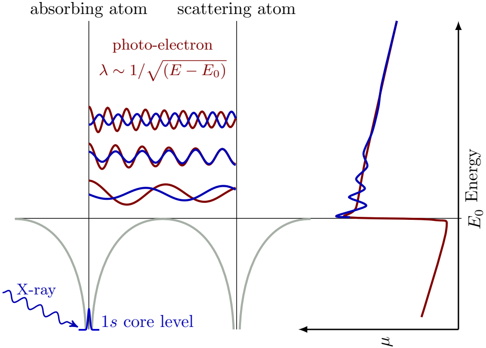

The photo-electron scattered back will interfere with itself.

μ depends on the presence of an electron state with energy $(E - E_0)$, at the absorbing atom.

The scattered photoelectron partially fills that state.

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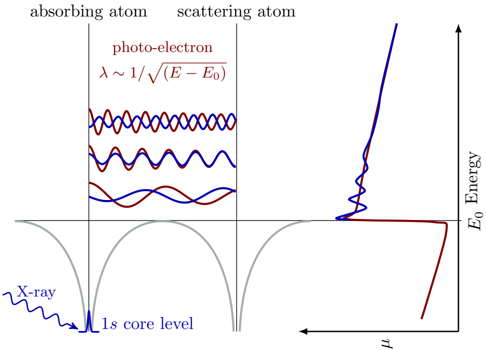

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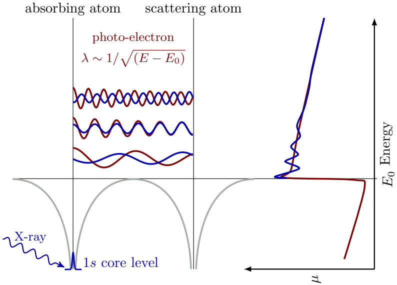
XAFS oscillations are due to the interference of the outgoing photo-electron with the photo-electron scattered from neighboring atoms.

X-ray Absorption: Fermi's Golden Rule

Going back to our definition

$$\mu(E) = \mu_0(E)[1 + \chi(E)]$$

we'll work out a form of the EXAFS Equation for $\chi(k)$ to use in analysis.



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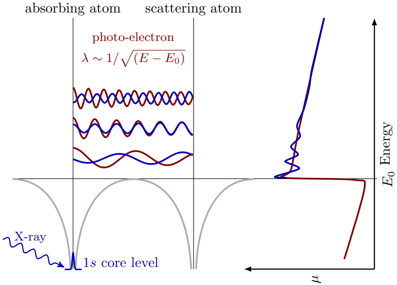

Fermi's Golden Rule describes $\mu(E)$ as a transition between quantum states:

$$\mu(E) \sim |\langle i|\mathcal{H}|f\rangle|^2$$

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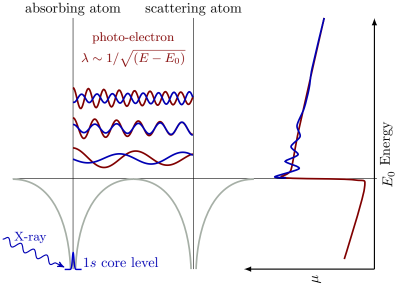

Fermi's Golden Rule describes $\mu(E)$ as a transition between quantum states:

$$\mu(E) \sim |\langle i|\mathcal{H}|f\rangle|^2$$

$\langle i|$ the *initial state* has a core level electron and the photon.
This is not altered by the neighboring atom.

$\mathcal{H}$ the *interaction*. In the dipole approximation, $\mathcal{H} = e^{ikr} \approx 1$.

$|f\rangle$ the *final state* has a photo-electron, a hole in the core, and no photon.
This is altered by the neighboring atom: *the photo-electron scatters*.

μ and χ and the photo-electron wavefunction

Writing $|f\rangle = |f_0 + \Delta f\rangle$, where Δf gives the change in photo-electron final state due to backscattering from the neighboring atom, we can expand μ to get

$$\mu(E) \sim |\langle i|\mathcal{H}|f_0\rangle|^2 [1 + \frac{\langle i|\mathcal{H}|\Delta f\rangle\langle f_0|\mathcal{H}|i\rangle^*}{|\langle i|\mathcal{H}|f_0\rangle|^2} + C.C]$$

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$$\begin{array}{rcl} \mu_0(E) \sim & |\langle i|\mathcal{H}|f_0\rangle|^2 & [\text{atomic background}] \\ \chi(E) \sim & \langle i|\mathcal{H}|\Delta f\rangle \sim \langle i|\Delta f\rangle & [\text{XAFS oscillations}] \end{array}$$

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The *initial state* – the core-level electron – is highly localized at the center of the absorbing atom, it is nearly a δ-function:

$$\chi \sim \langle i|\Delta f\rangle \sim \int dr \delta(r)\psi_{\rm scatt}(r) = \psi_{\rm scatt}(r = 0).$$

χ is the amplitude of the portion of the photo-electron wave-function that was scattered by the neighboring atoms **at the absorbing atom**.

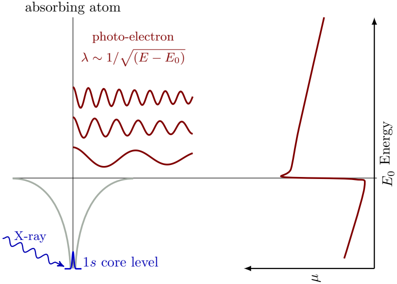
The EXAFS Equation: simple description

With $\chi \sim \psi_{\rm scatt}(0)$, We'll start with a spherical wave function for the photo-electron

$$\psi(k, r) = e^{ikr}/kr$$

we can model $\chi(k)$ as the photo-electron

1. leaves the absorbing atom



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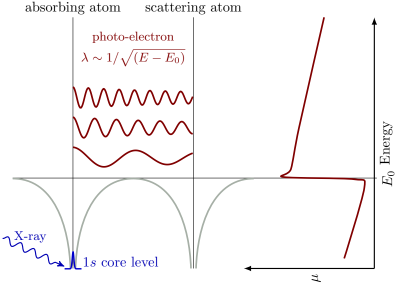

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where scattering from the neighboring atom gives:

$f(k)$	the scattering amplitude for the atom.
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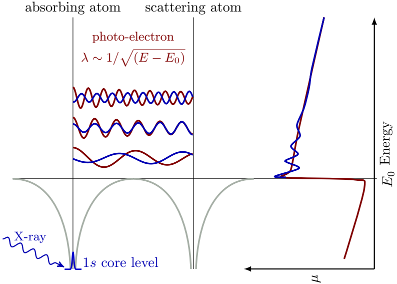
1. leaves the absorbing atom
2. scatters from the neighbor atom
3. returns to the absorbing atom



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turning complex number into real numbers gives the EXAFS Equation. . .

Development of the EXAFS Equation

$$\chi(k) = \frac{f(k)}{kR^2} \sin[2kR + \delta(k)]$$

The EXAFS Equation for 1 scattering atom.

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The EXAFS Equation for 1 scattering atom.

For N neighboring atoms, and with thermal and static disorder of σ^2, giving the *mean-square disorder* in R, we have

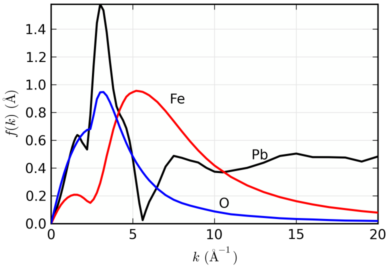
$$\chi(k) = \frac{Nf(k)e^{-2k^2\sigma^2}}{kR^2}\sin\left[2kR + \delta(k)\right]$$

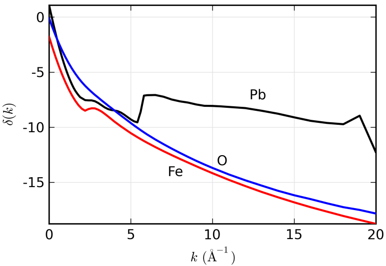
A real system has atoms at different distances and of different types. We add all these contributions to get a better version of the EXAFS equation:

$$\chi(k) = \sum_j \frac{N_j f_j(k) e^{-2k^2\sigma_j^2}}{k{R_j}^2}\sin[2kR_j + \delta_j(k)]$$

Scattering Amplitude and Phase-Shift

The scattering amplitude $f(k)$ and phase-shift $\delta(k)$ depend on atomic number.





$f(k)$ extends to higher k values for higher Z elements. For very heavy elements, there is structure in $f(k)$.

$\delta(k)$ shows sharp changes for very heavy elements. These functions can be calculated for modeling EXAFS.

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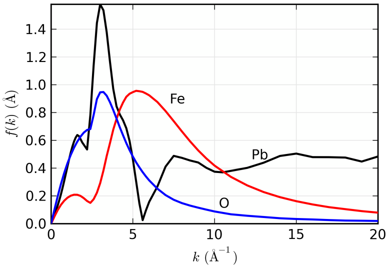

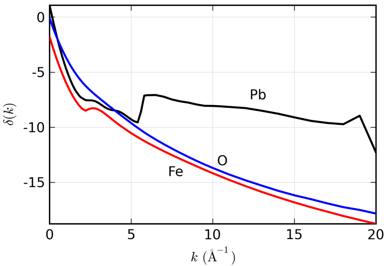

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$\delta(k)$ shows sharp changes for very heavy elements. These functions can be calculated for modeling EXAFS.

These complex factors allow EXAFS to distinguish the species of neighboring atom:

Z can usually be determined to ±5.
Fe and O can be distinguished, but not Fe and Mn.

The EXAFS Equation: What we left out

This simple description so far is qualitatively right, but for quantitative EXAFS calculations, it's important to consider several other points:

Inelastic Losses	Processes that alter the absorbing atom or photo-electron before the photo-electron scatters back home.
Extrinsic Losses	photo-electron mean-free path, including complex self-energy and finite core-hole lifetime.
Intrinsic Losses	relaxation of absorbing atom due to the presence of the core hole.
Multiple Scattering	the photo-electron can scatter multiple times, which is important at low k, and can be important at high k for some systems.

Caclulations *should* include these effects, and mostly do.

We'll discuss these in more detail . . . .

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Photo-Electron Mean-Free Path (extrinsic losses)

To get to

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we used a spherical wave for the photo-electron:

$$\psi(k, r) \sim e^{ikr}/kr$$

But this ignores two things:

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But this ignores two things:

1. The photo-electron can also scatter *inelastically*, and may not be able to get back the absorbing atom in tact.
2. The hole in the core electron level has a *finite lifetime*, also limiting how far the photo-electron can go out and make it back to "the same" absorbing atom.

A *mean free path* (λ) describes how far the photo-electron can go before it scatters, losing energy to other electrons, phonons, etc.

Photo-Electron Mean-Free Path

To account for the mean-free-path, we can replace the spherical photo-electron wavefunction:

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with a damped wave-function:

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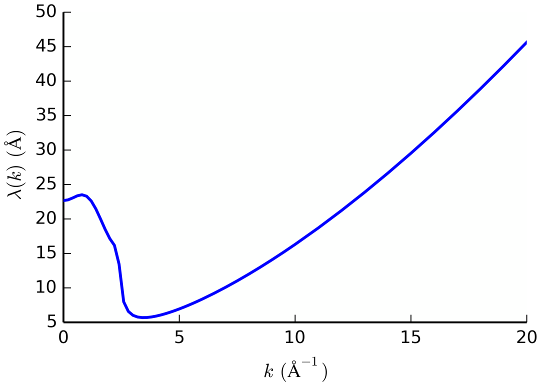
Photo-Electron Mean-Free Path: nearly universal shape



λ is mostly independent of the system, and depends strongly on k:

- For $3\,\mathrm{Å}^{-1} < \mathrm{k} < 15\,\mathrm{Å}^{-1}$, $\lambda < 30\,\mathrm{Å}$
- This (and the R^{-2} term) makes EXAFS a *local atomic probe*.
- For XANES ($k < 2\,\mathrm{Å}^{-1}$) Both λ and R^{-2} get large: XANES is not really a *local probe*.

S_0^2: Amplitude Reduction Term (intrinsic losses)

Another important correction that we left out so far:

The Amplitude Reduction Term is due to the relaxation of the *other electrons in the absorbing atom* to the hole in the core level:

$$S_0^2 = |\langle \Phi_f^{N-1} | \Phi_0^{N-1} \rangle|^2$$

$|\Phi_0^{N-1}\rangle = (N-1)$ electrons in unexcited atom.
$\langle \Phi_f^{N-1}| = (N-1)$ electrons, relaxed by core-hole.

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$|\Phi_0^{N-1}\rangle = (N-1)$ electrons in unexcited atom.
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and is used as a Fitting Parameter that multiplies χ:

S_0^2: Amplitude Reduction Term (intrinsic losses)

Another important correction that we left out so far:

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S_0^2 is Completely Correlated with N (!!!)

S_0^2 – along with normalization of spectra – makes EXAFS amplitudes (and therefore N) less precise than EXAFS phases (and therefore R).

The EXAFS Equation: Sum over Scattering Paths

We need some way to account for different neighbor species (Fe-O, Fe-Fe):

$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)} \, e^{-2k^2\sigma_j^2}}{k{R_j}^2} \sin\left[2kR_j + \delta_j(k)\right]$$

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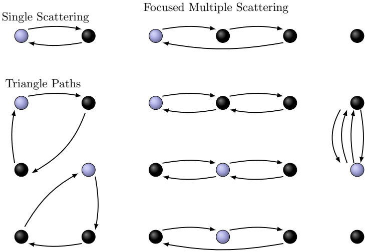


Triangle Paths with angles $45 < \theta < 135^\circ$ aren't strong, but there can be a lot of them.

Linear paths with angles $\theta \approx 180^\circ$, are very strong: the photo-electron can be focused through one atom to the next.

Scattering is strongest when $\theta > 150^\circ$.

This can be used to measure bond angles.

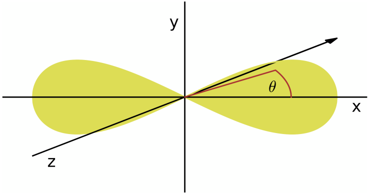
For first shell analysis, multiple scattering is hardly ever needed.

X-ray Polarization

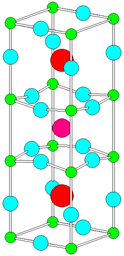
A synchrotron is highly polarized ($> 99.9\%$) in the horizontal plane.

A photo-electron from a *K* shell goes as a *p* orbital ($\cos^2\theta$), mostly in the horizontal plane.

It *never* sees atoms in the vertical (y) plane or along the beam direction (z).



For anisotropic systems (surfaces, non-cubic crystals, . . .) this can be important: It can be either confounding or useful!



Anistropy of the *crystal* doesn't really matter – anisotropy in the *local structure* does.

A sorbed ion on a surface, or ion intercalated in a layered material, may show very strong polarization dependence.

Structural Disorder and the Pair Distribution Function

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- Each absorbed x-ray generates 1 photo-electron.
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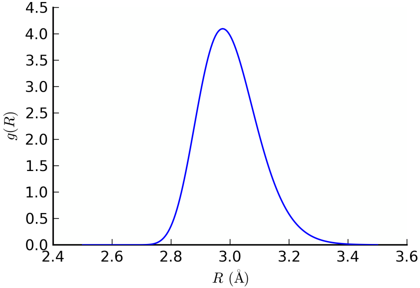
More generally, EXAFS samples the

Partial Pair Distribution Function

$g(R)$ = probability that an atom is a distance R away from the absorber.

For now, we'll just note that this may need to be taken into account.



The EXAFS Equation: Recap

Even with all those complications and caveats, we still use the *EXAFS Equation*:

$$\chi(k) = \sum_j \frac{N_j f_j(k) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{k{R_j}^2} \sin[2kR_j + \delta_j(k)]$$

where $f(k)$ and $\delta(k)$ are *photo-electron scattering properties* of the neighboring atom and $\lambda(k)$ is the photo-electron mean-free-path.

Again, if we know these properties, we can determine:

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σ^2	mean-square disorder of neighbor distance (or more complicated disorder terms).

$f(k)$ and $\delta(k)$ depend on atomic number Z of the scattering atom, so we can also determine the species of the neighboring atom.

EXAFS Theory: Conclusions

We have an EXAFS Equation that we can use to model EXAFS data.

$$\chi(k) = \sum_j \frac{N_j f_j(k) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{k{R_j}^2} \sin[2kR_j + \delta_j(k)]$$

In later videos and demos we'll show how to use this for analyzing EXAFS data.

More information on X-rays and X-ray Absorption Spectroscopy:

https://xafs.xrayabsorption.org/

Fundamentals of XAFS M. Newville, Reviews in Mineralogy & Geochemistry **78**, 2014.

Introduction to XAFS G. Bunker, Cambridge Univ Press, 2010.

XAFS for Everyone S. Calvin, CRC Press, 2013.

Elements of Modern X-ray Physics J. Als-Nielsen & D. McMorrow, John Wiley & Sons. 2001