Today's outline - April 09, 2020 (part A)

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Homework Assignment #06:
Chapter 6: 1,6,7,8,9
due Tuesday, April 14, 2020

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Homework Assignment #06:
Chapter 6: 1,6,7,8,9
due Tuesday, April 14, 2020

Homework Assignment #07:
Chapter 7: 2,3,9,10,11
due Thursday, April 23, 2020

Resonant scattering from a single electron

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$$f'_s = \frac{\omega_s^2(\omega^2 + \omega_s^2)}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2}$$

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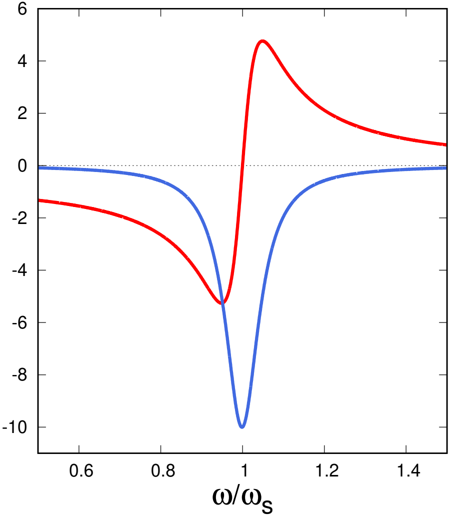

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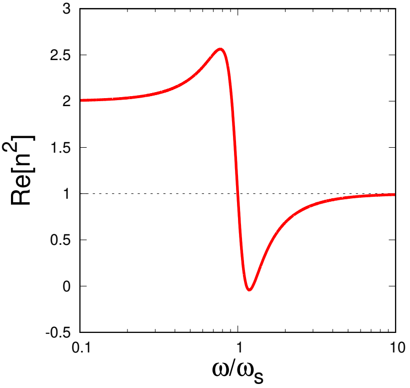

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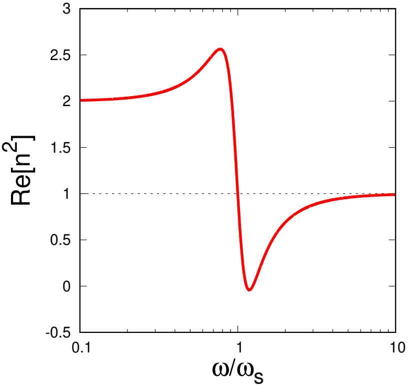

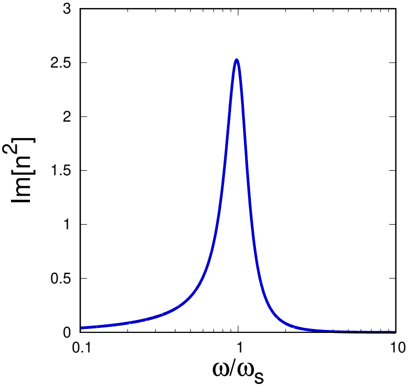

Absorption cross-section

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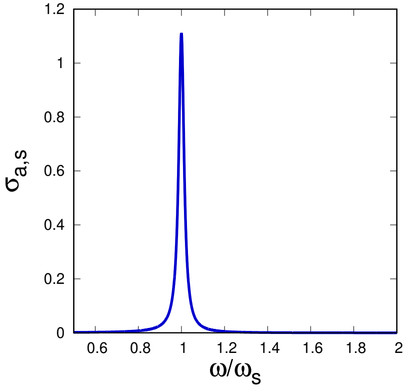

$$\sigma_{a,s}(\omega) = 4\pi r_0 c \frac{\omega_s^2 \Gamma}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2}$$

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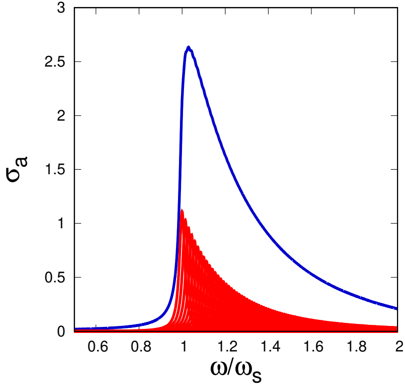

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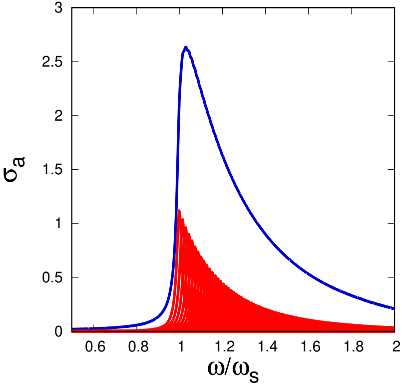

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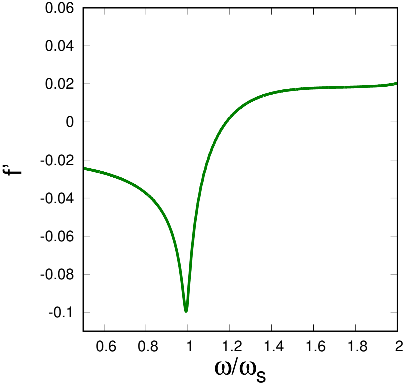

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The Kramers-Kronig relations are derived using Cauchy's theorem to integrate a function with a pole

More about Kramers-Kronig

The Kramers-Kronig relations can be rewritten by multiplying top and bottom by $(\omega' + \omega)$

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The Kramers-Kronig relations can be rewritten by multiplying top and bottom by $(\omega' + \omega)$ and noting that f'' is odd

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this can be evaluated for two $1s$ electrons

Computing f'

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For 2 1s electrons

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For 2 1s electrons

$$\sigma_a(1) = 2\left(\frac{256\pi}{3e^4}\right)\lambda_K r_0$$

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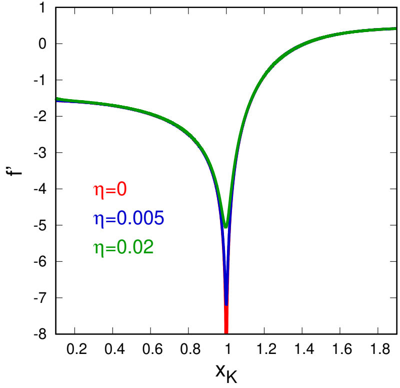

Computing f'

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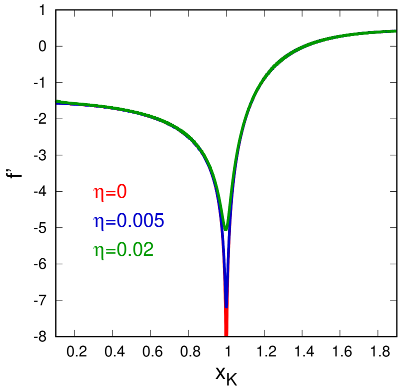

at high energies ($x_K \to \infty$) this dispersion correction vanishes as expected and at low energies ($x_K, q \to 0$) the correction is -1.565, thereby partially quenching the scattering from the two 1s electrons

Self-consistent cross-section calculations

More accurate calculations of the resonant corrections to the scattering factor can be made using a full quantum mechanical treatment

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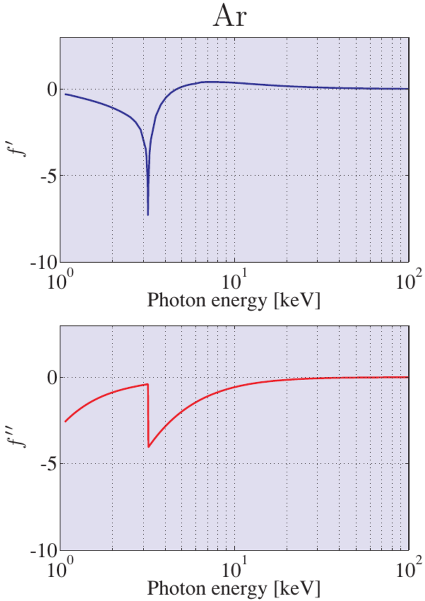
The simple model, however, reproduces the main features of the Ar K-edge



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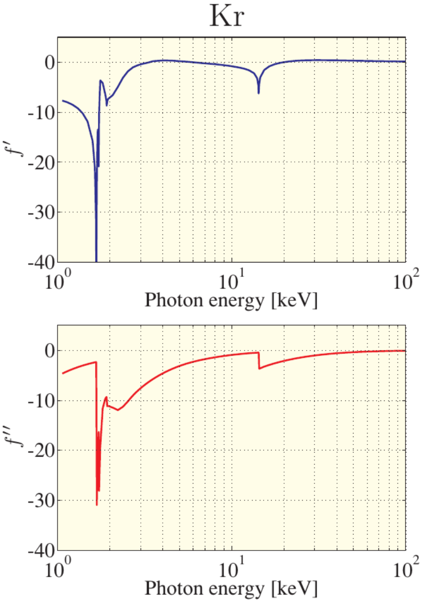

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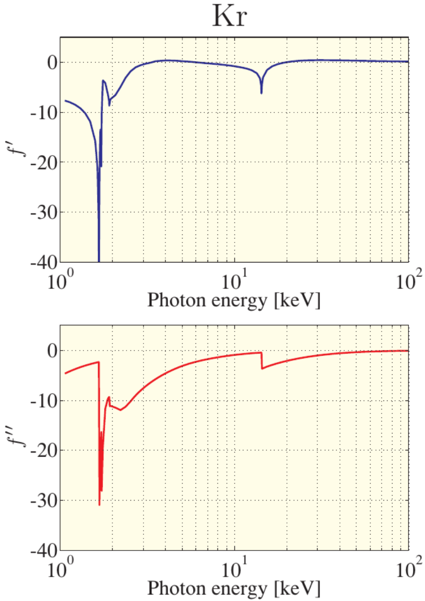
What is lacking, even in the more sophisticated calcuations, are the resonances near the absorption edges due to XANES, EXAFS and other localized resonance phenomena



Today's outline - April 09, 2020 (part B)

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- Friedel's Law

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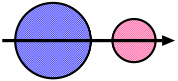
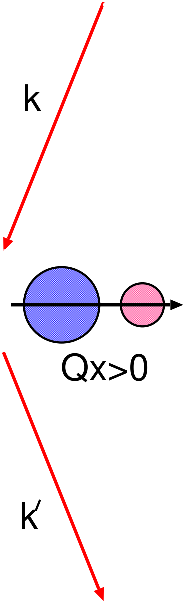
- Bijvoet (Bay-voot) Pairs

Scattering from two unlike atoms



Two unlike atoms with scattering factors f_1 and f_2 are oriented by a vector pointing from the larger to the smaller.

Scattering from two unlike atoms



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Consider two cases, with the scattering vector Q

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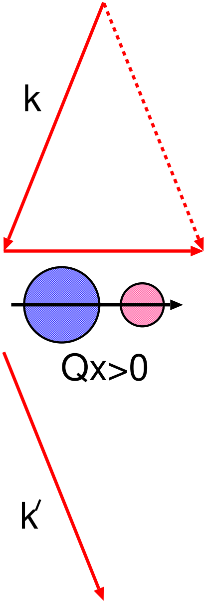

Two unlike atoms with scattering factors f_1 and f_2 are oriented by a vector pointing from the larger to the smaller.

Consider two cases, with the scattering vector Q in the same direction as the orientation vector

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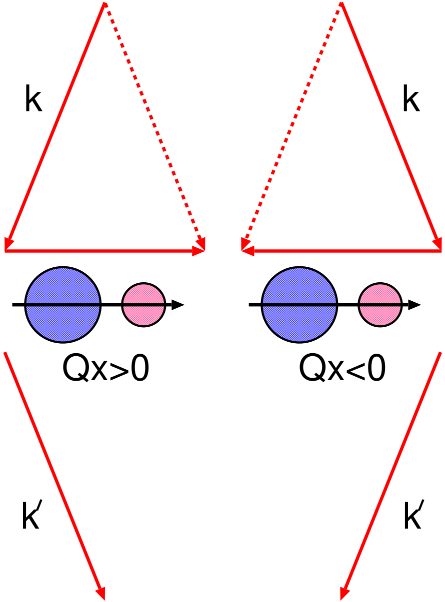

Two unlike atoms with scattering factors f_1 and f_2 are oriented by a vector pointing from the larger to the smaller.

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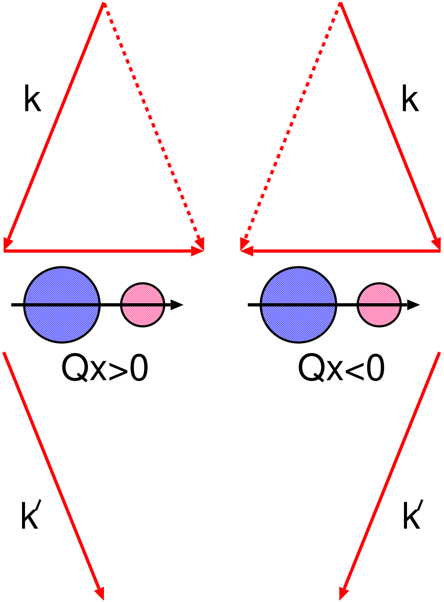
Scattering from two unlike atoms



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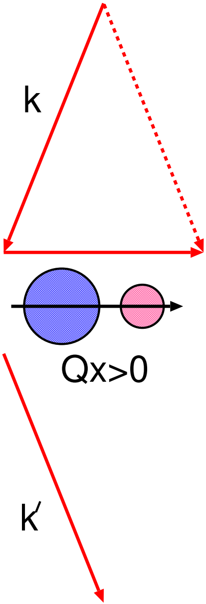
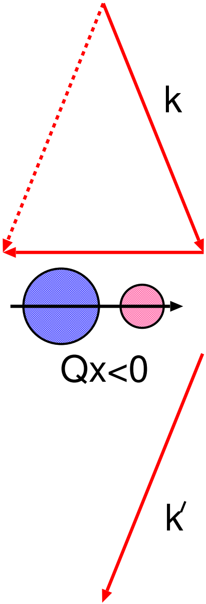
Now compute the scattered intensity in each case, assuming scattering factors are purely real.

Friedel's Law





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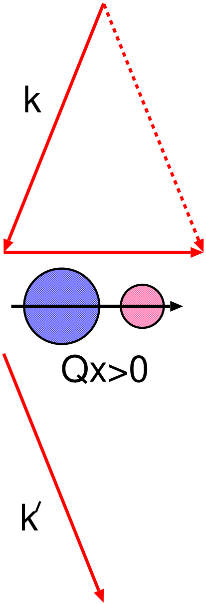
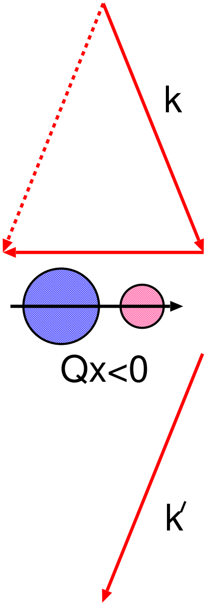
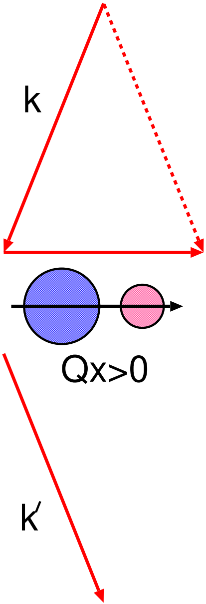


$$A(+Q) = f_1 + f_2 e^{+iQx}$$



Friedel's Law



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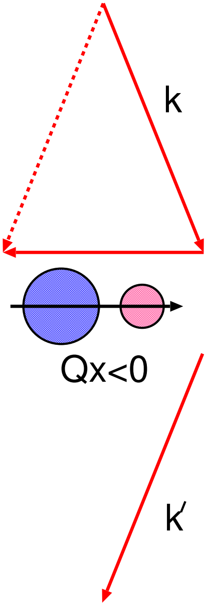

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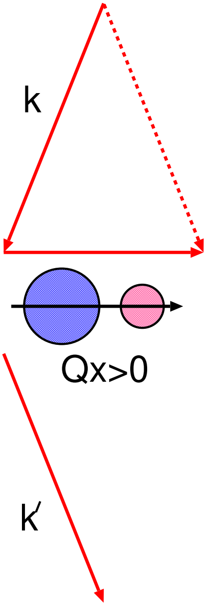

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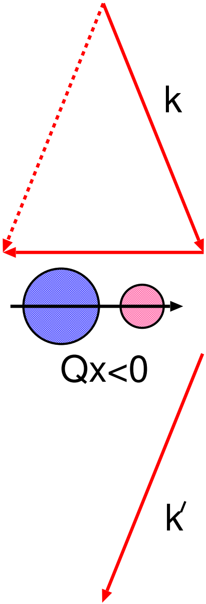

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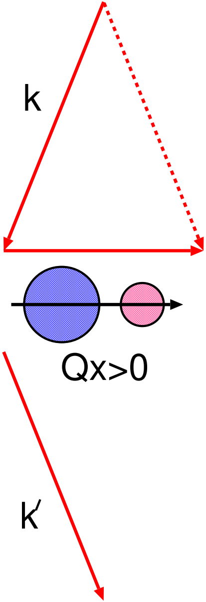

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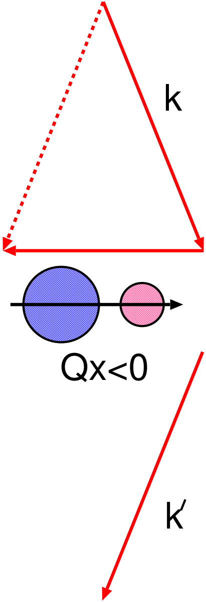

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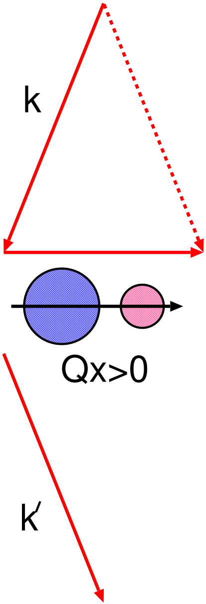

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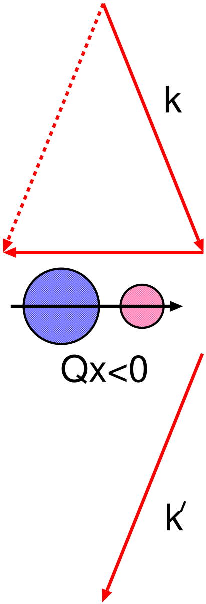

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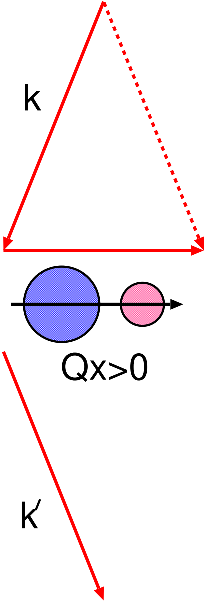

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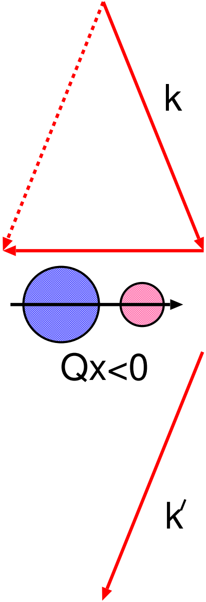

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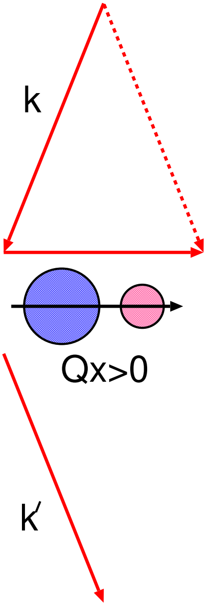

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$I(+Q) = I(-Q)$ Friedel's Law

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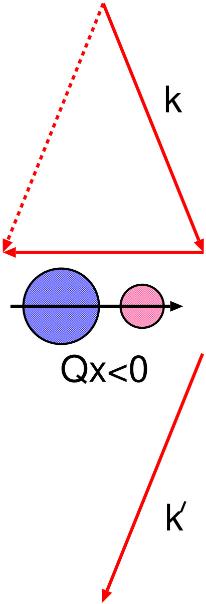

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and the two intensities are no longer equal, breaking Friedel's Law

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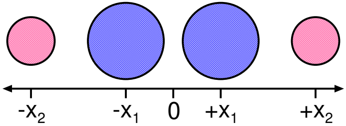

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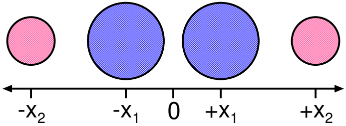

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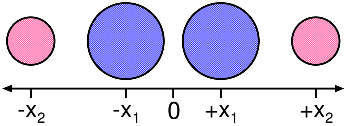

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$$F = r_1 e^{-i(\phi_1 + Qx_1)} + r_1 e^{-i(\phi_1 - Qx_1)} + r_2 e^{-i(\phi_2 + Qx_2)} + r_2 e^{-i(\phi_2 - Qx_2)}$$

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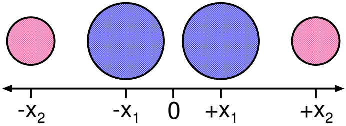

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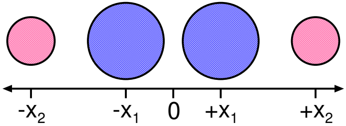

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$$= [2r_1 \cos(Qx_1)]e^{-i\phi_1} + [2r_2 \cos(Qx_2)]e^{-i\phi_2}$$

$$I(Q) = 4|f_1|^2 \cos^2(Qx_1) + 4|f_2|^2 \cos^2(Qx_2)$$
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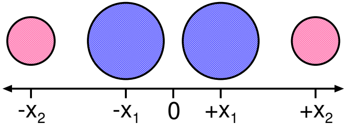
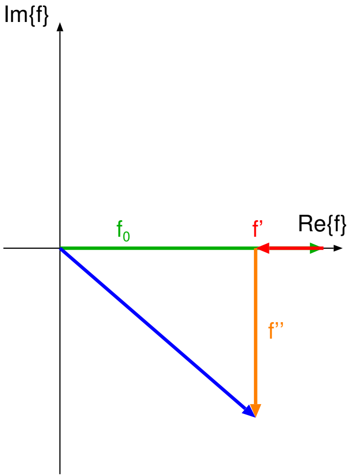


$$\begin{aligned} F &= r_1 e^{-i(\phi_1 + Qx_1)} + r_1 e^{-i(\phi_1 - Qx_1)} + r_2 e^{-i(\phi_2 + Qx_2)} + r_2 e^{-i(\phi_2 - Qx_2)} \\ &= [2r_1 \cos(Qx_1)] e^{-i\phi_1} + [2r_2 \cos(Qx_2)] e^{-i\phi_2} \end{aligned}$$

$$\begin{aligned} I(Q) = 4|f_1|^2 \cos^2(Qx_1) + 4|f_2|^2 \cos^2(Qx_2) \\ + 8|f_1||f_2| \cos(Qx_1)\cos(Qx_2)\cos(\phi_2 - \phi_1) = I(-Q) \end{aligned}$$

Argand diagram

This can all be described graphically using an Argand (phasor) diagram:



build the scattering vector from real and imaginary components with the imaginary part always $\pi/2$ clockwise compared to the real part

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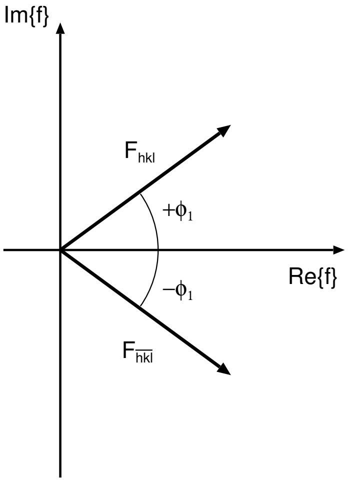

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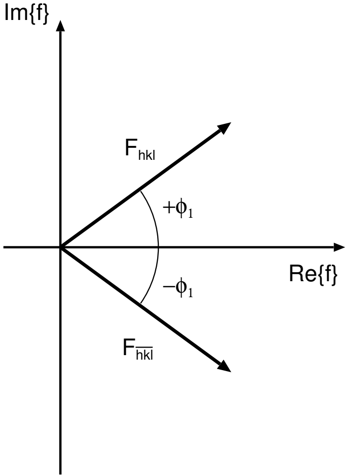

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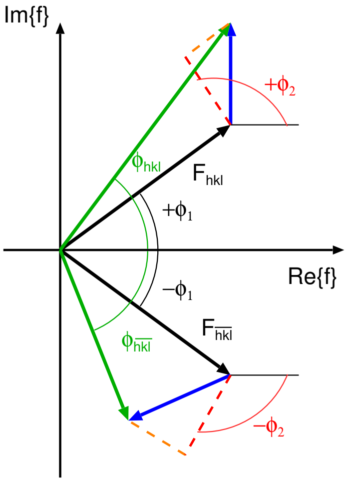

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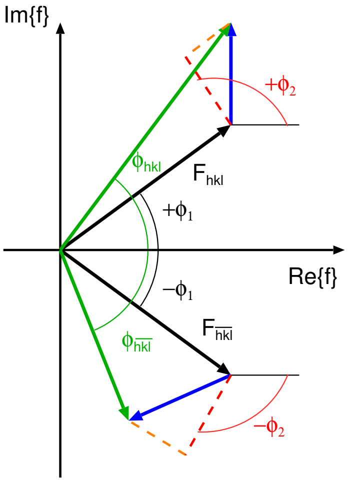

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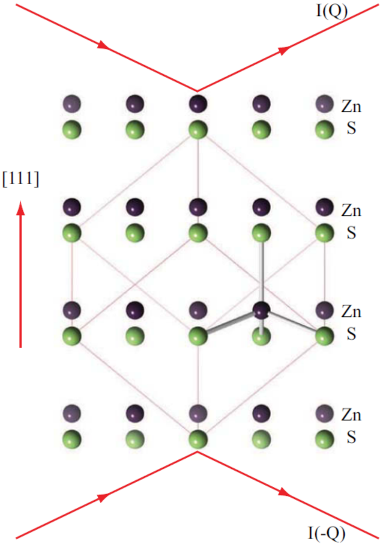
the scattering vectors now have different magnitudes and phases

ZnS example



The ZnS structure is not centrosymmetric and when viewed along the ⟨111⟩ direction, it shows alternating stacked planes of Zn and S atoms.

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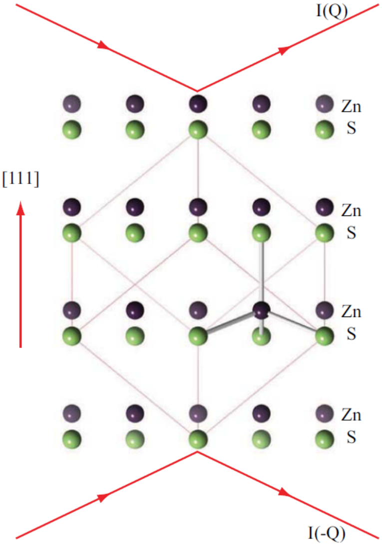
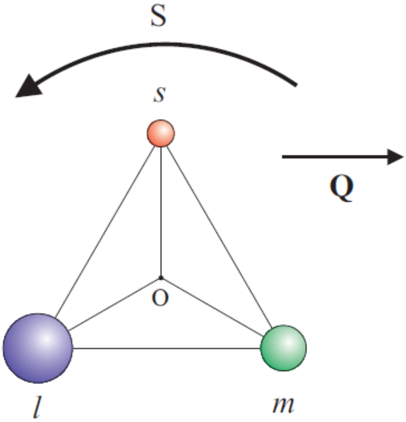


The ZnS structure is not centrosymmetric and when viewed along the $\langle 111 \rangle$ direction, it shows alternating stacked planes of Zn and S atoms.

Scattering from opposite faces of a single crystal of ZnS gives a different scattering factor and one can deduce the terminating surface atom.

Bijvoet pairs - chiral molecules

Consider a tetrahedral molecule of carbon with four different species at each corner, oriented so the lightest is projected to the origin.



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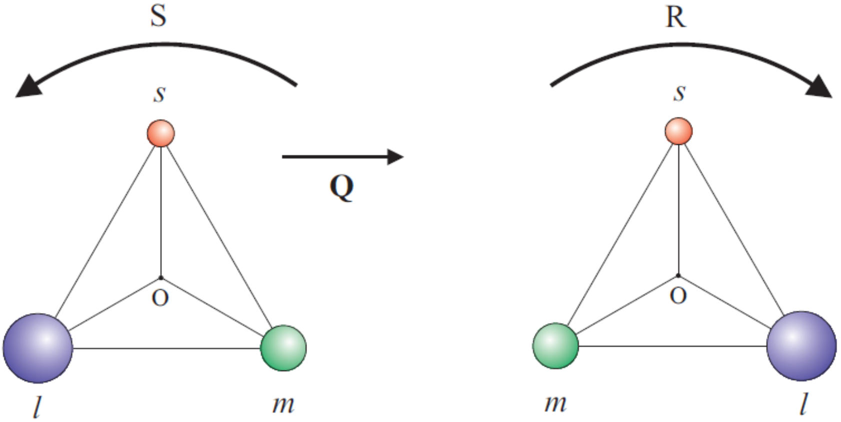
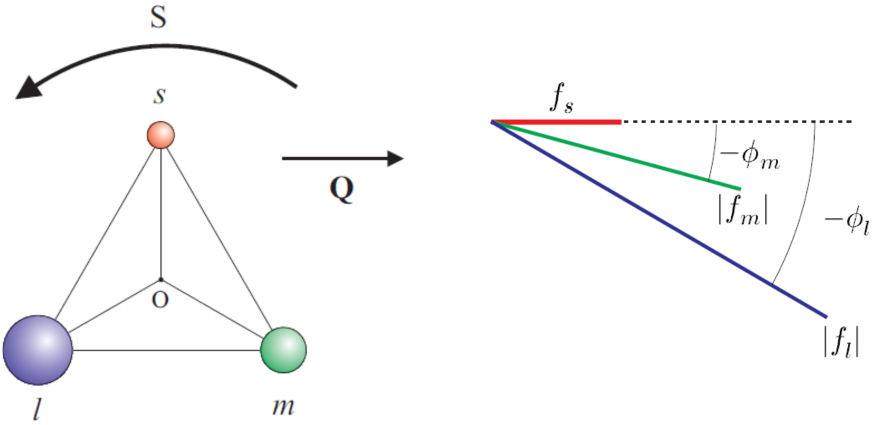
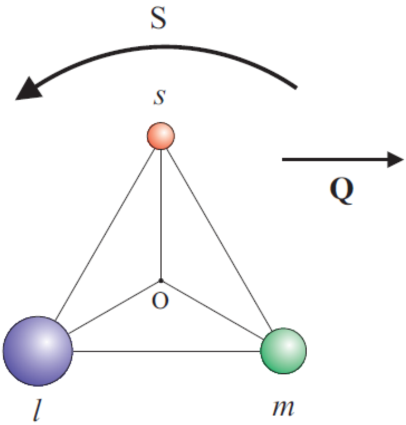


Each of the three atoms not at the origin has a scattering factor for $\vec{Q}$ as shown



Left handed scattering factor



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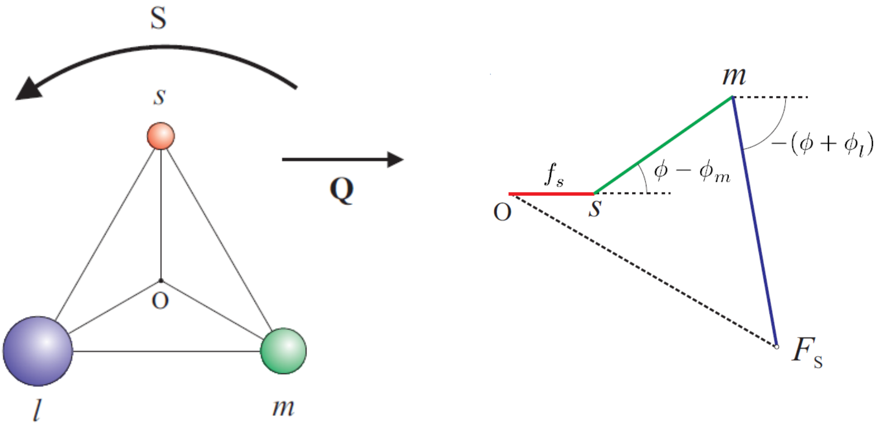
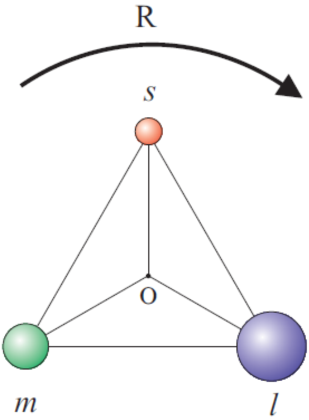


$$F_S = |f_s| + |f_m|e^{-i\phi_m}e^{i\phi} + |f_l|e^{-i\phi_l}e^{-i\phi}$$

Right handed scattering factor



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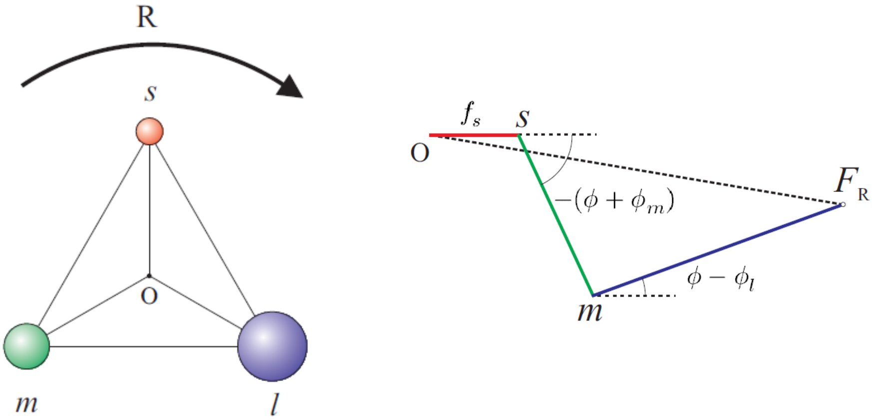
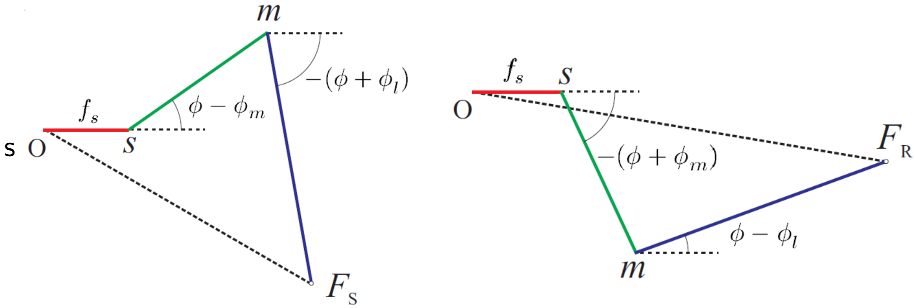


$$F_R = |f_s| + |f_m|e^{-i\phi_m}e^{-i\phi} + |f_l|e^{-i\phi_l}e^{i\phi}$$

Scattering factor comparison

It is thus possible to tell the difference in handedness of chiral molecule simply by x-ray scattering



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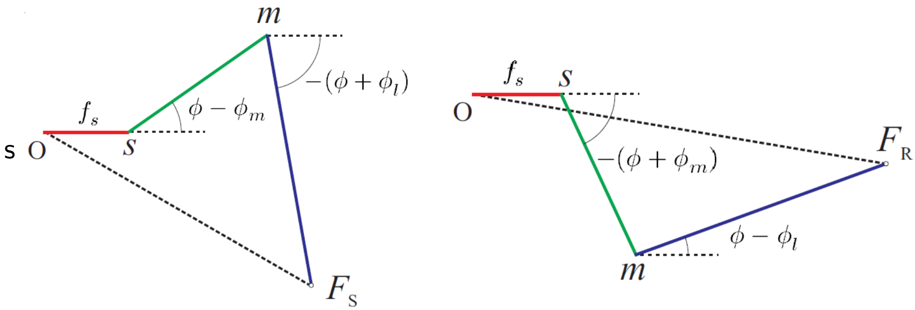

$$\left| |f_s| + |f_m| e^{-i\phi_m} e^{i\phi} + |f_l| e^{-i\phi_l} e^{-i\phi} \right|^2 \neq \left| |f_s| + |f_m| e^{-i\phi_m} e^{-i\phi} + |f_l| e^{-i\phi_l} e^{i\phi} \right|^2$$

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Multi-wavelength anomalous dispersion phasing is a technique commonly used in protein crystallography to help solve the "phase problem"

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Atoms with an absorption edge in the energy range being scanned have a scattering factor

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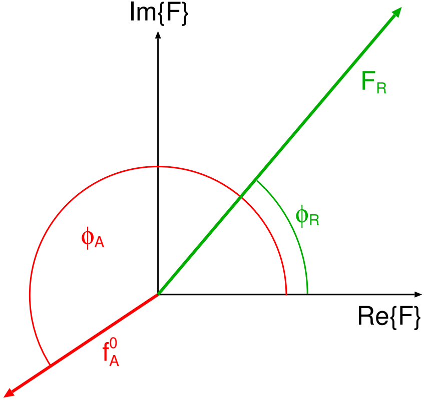

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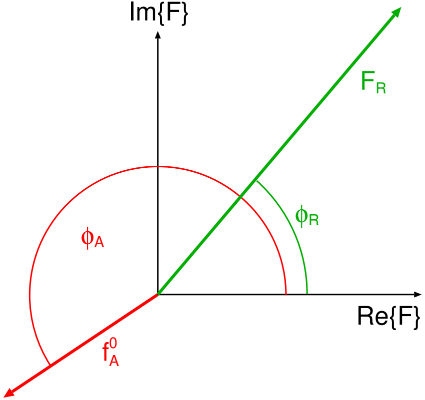

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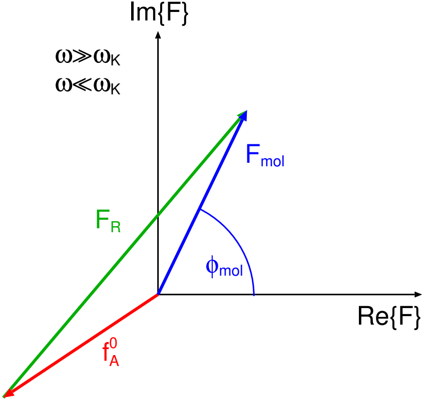
At energies far away from the absorption edge, the scattering factors of the anomalous atoms with angle ϕ_A and the rest of the molecule with angle ϕ_R add vectorially in an Argand diagram to give the molecule scattering factor F_{mol} with phase angle ϕ_{mol}



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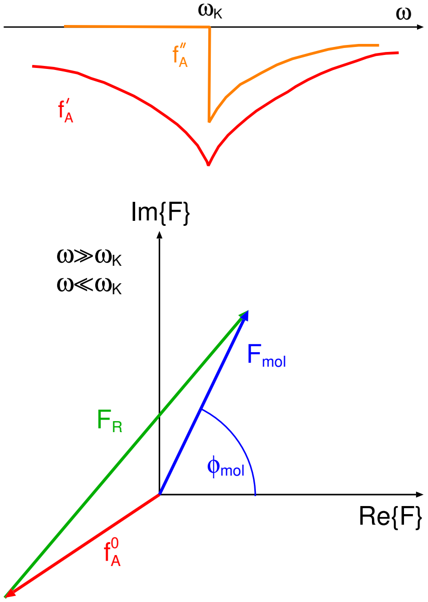

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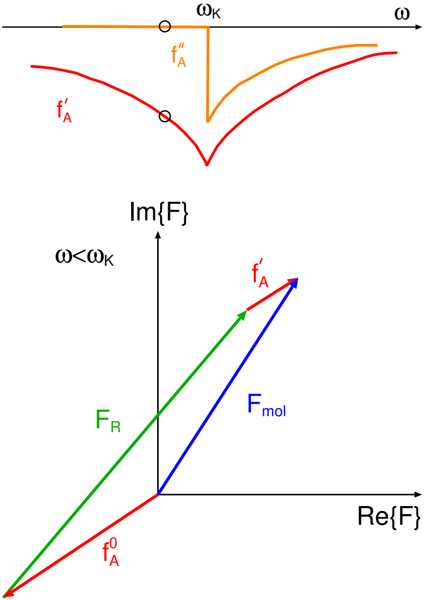
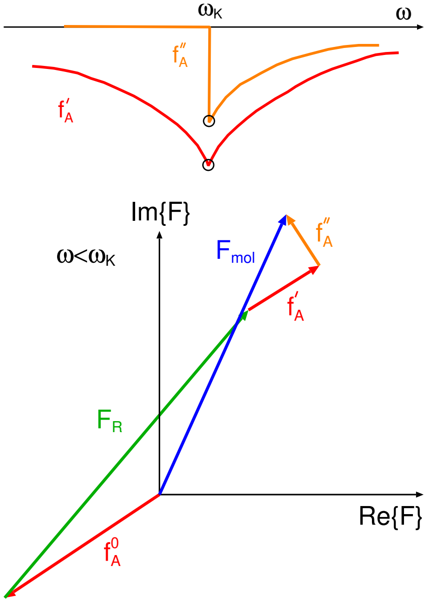


As the x-ray energy approaches the absorption edge, a resonant term f_A' grows with opposite sign from f_A^0 but there is no dissipative term

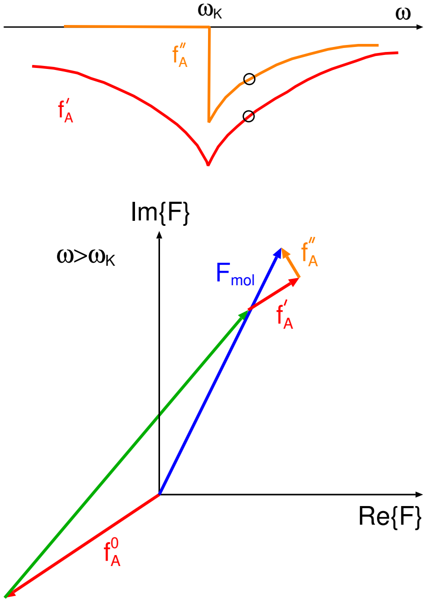
Multi-wavelength anomalous dispersion



As the x-ray energy approaches the absorption edge, a resonant term f_A' grows with opposite sign from f_A^0 but there is no dissipative term

At the absorption edge, a large dissipative term, f_A'', appears with a $\pi/2$ phase shift compared to f_A'

Multi-wavelength anomalous dispersion

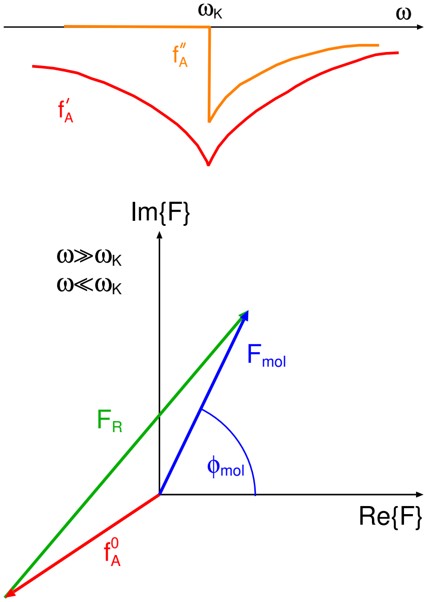


As the x-ray energy approaches the absorption edge, a resonant term f'_A grows with opposite sign from f^0_A but there is no dissipative term

At the absorption edge, a large dissipative term, f''_A, appears with a $\pi/2$ phase shift compared to f'_A

Once past the absorption edge both f'_A and f''_A shrink

Multi-wavelength anomalous dispersion



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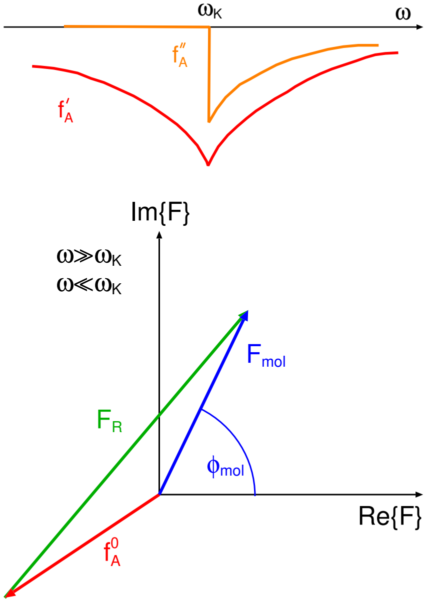
Once past the absorption edge both f_A' and f_A'' shrink eventually returning to zero at high energies

Multi-wavelength anomalous dispersion



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The change in the scattering factor of each Bragg reflection can be used to locate the position of the resonant atoms in the structure