Today's outline - September 28, 2021

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- Scattering review

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Reading Assignment: Chapter 4.3–4.4

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Reading Assignment: Chapter 4.3–4.4

Homework Assignment #03:
Chapter 3: 1,3,4,6,8
due Tuesday, October 05, 2021

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- Scattering review
- Kinematical scattering
- Liquid scattering

Reading Assignment: Chapter 4.3–4.4

Homework Assignment #03:
Chapter 3: 1,3,4,6,8
due Tuesday, October 05, 2021

Homework Assignment #04:
Chapter 4: 2,4,6,7.10
due Tuesday, October 19, 2021

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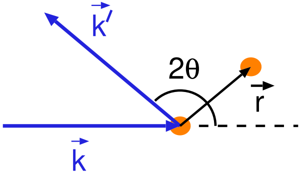

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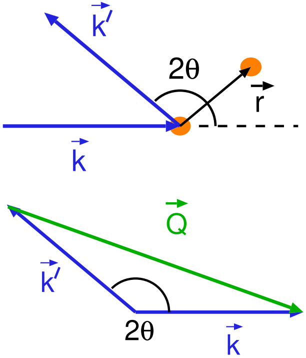

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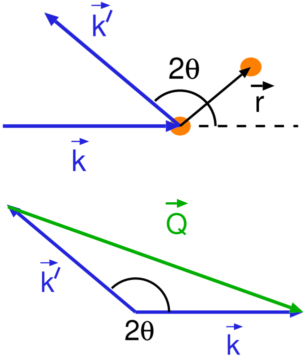

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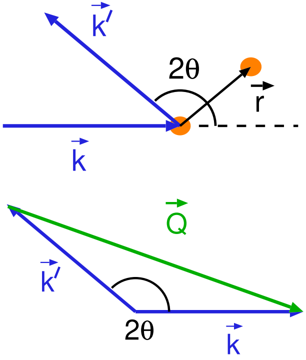

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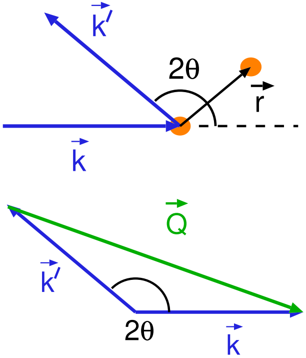

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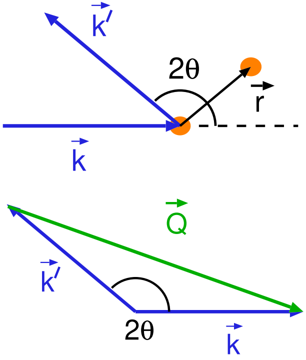

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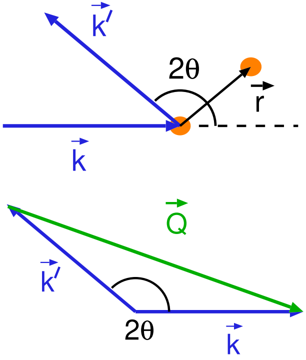

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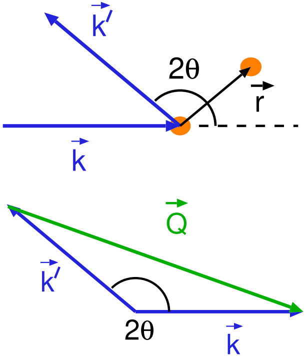

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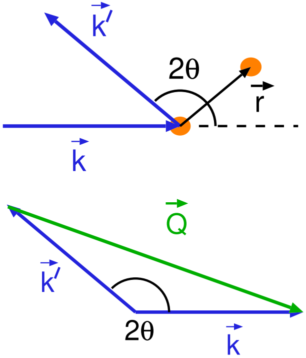

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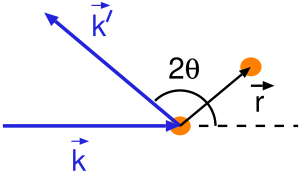

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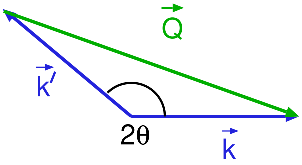

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Since experiments measure $I \propto A^2$, the phase information is lost. This is a problem if we don't know the specific orientation of the scattering system relative to the x-ray beam.

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We will now look at the consequences of this orientation and generalize to more than two electrons

Two electrons — fixed orientation

The expression

$$I(\vec{Q}) = 2r_0^2\left(1 + \cos(\vec{Q}\cdot\vec{r})\right)$$

assumes that the two electrons have a specific, fixed orientation. In this case the intensity as a function of Q is.

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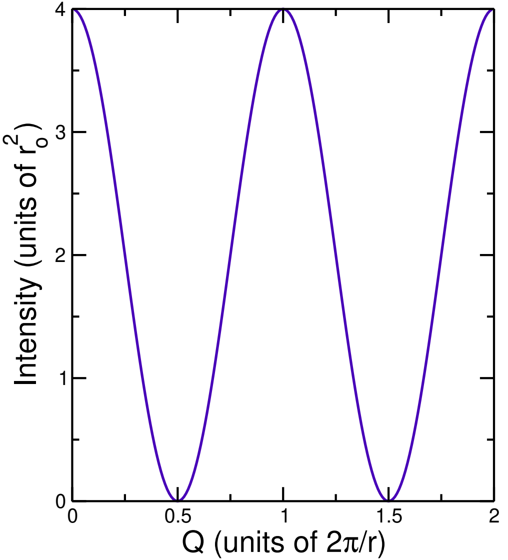

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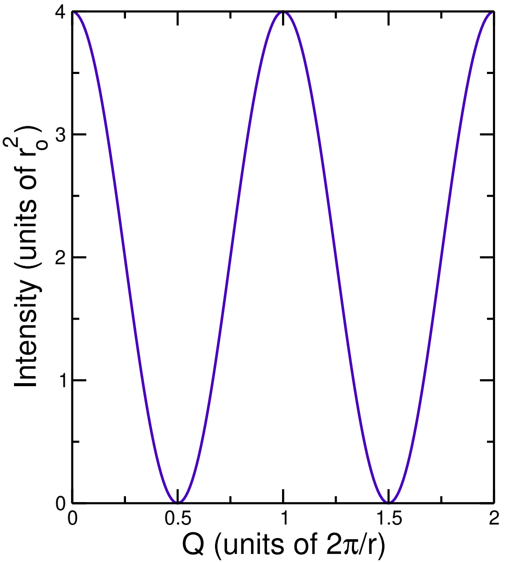
Fixed orientation is not the usual case, particularly for solution and small-angle scattering.



Orientation averaging

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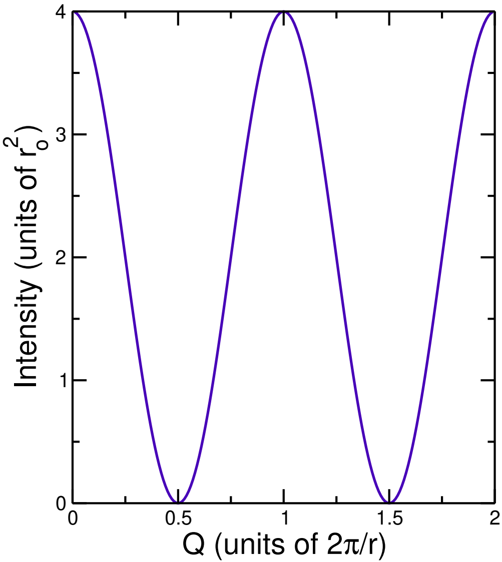

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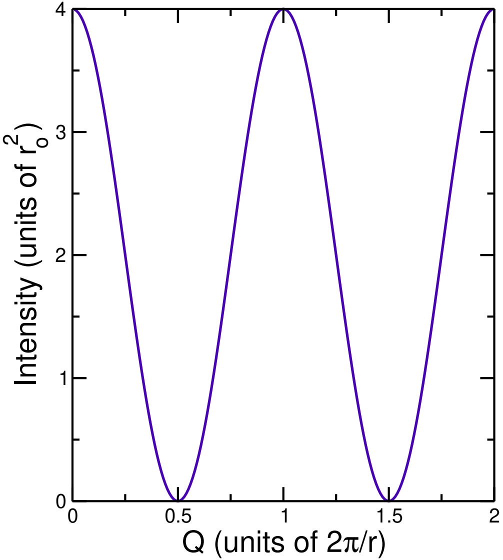

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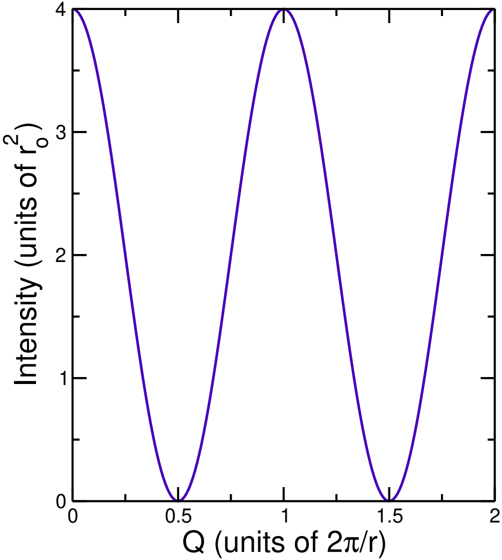

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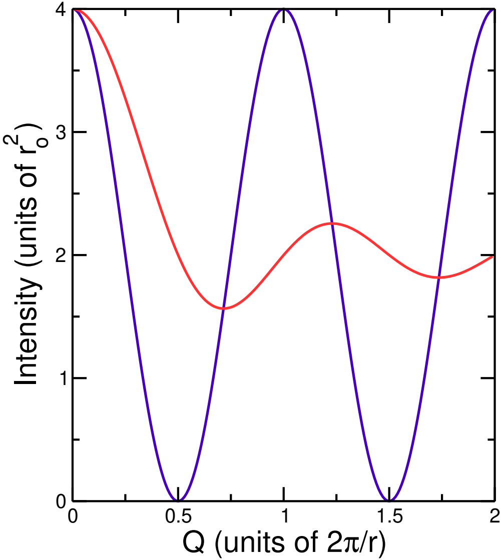

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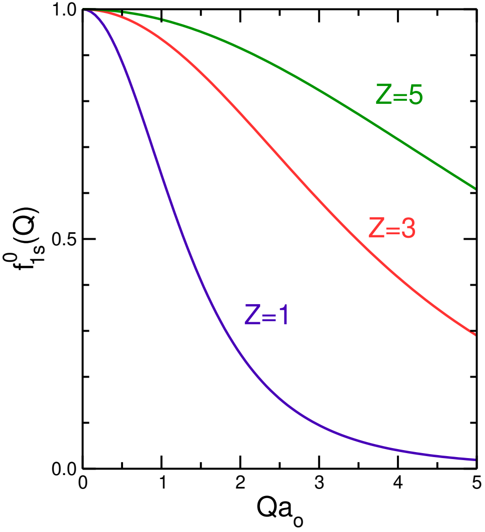

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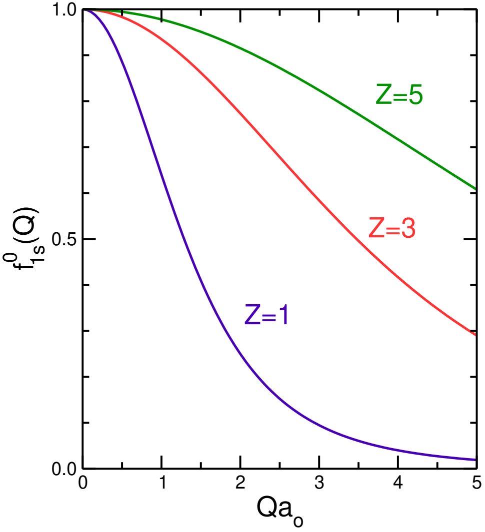

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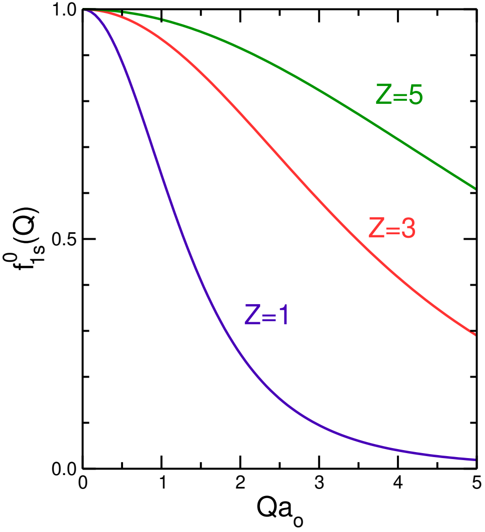

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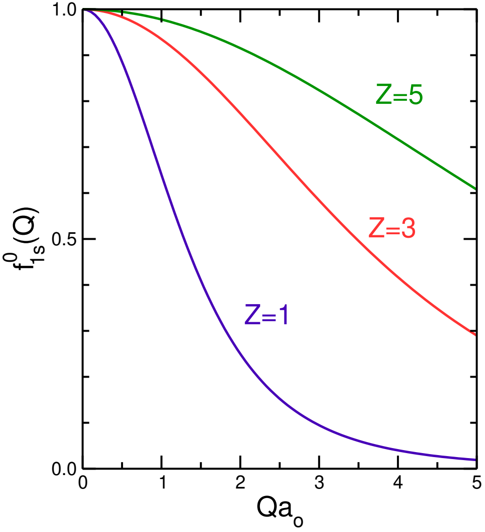

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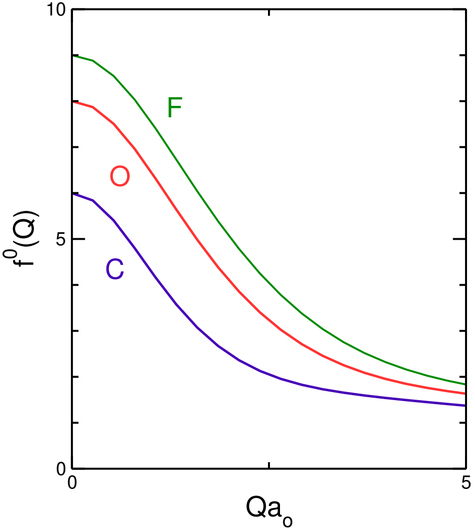

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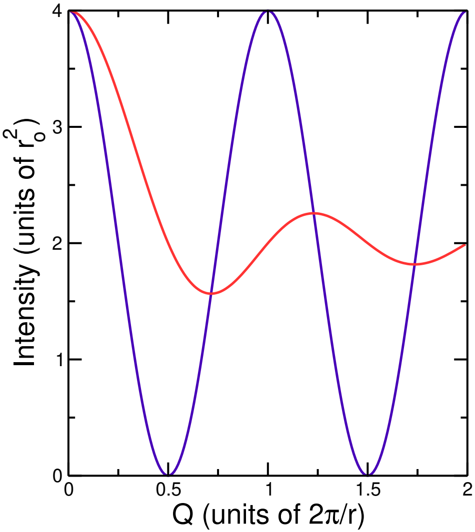

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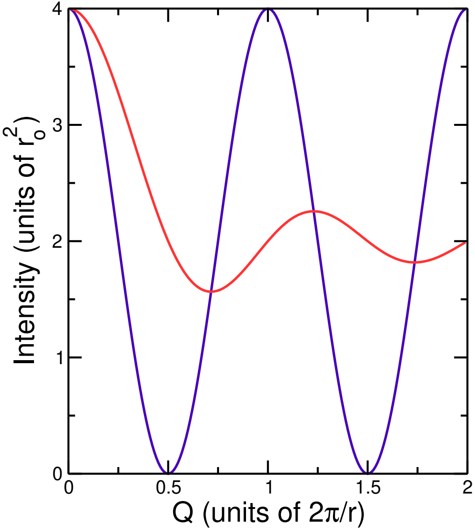

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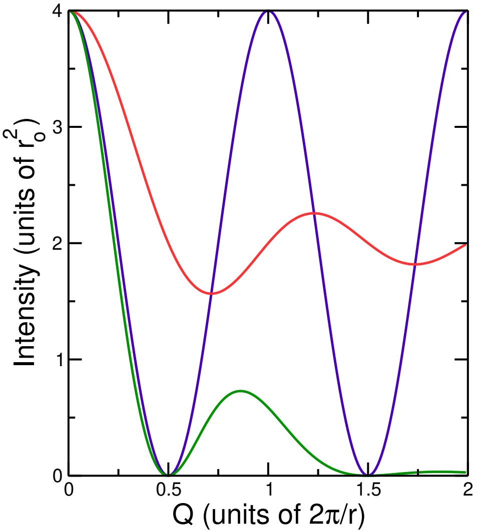

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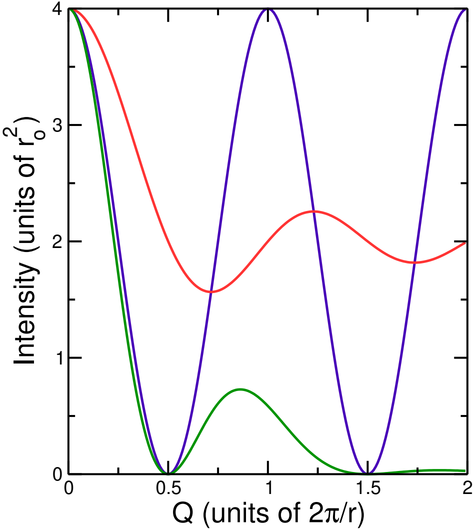

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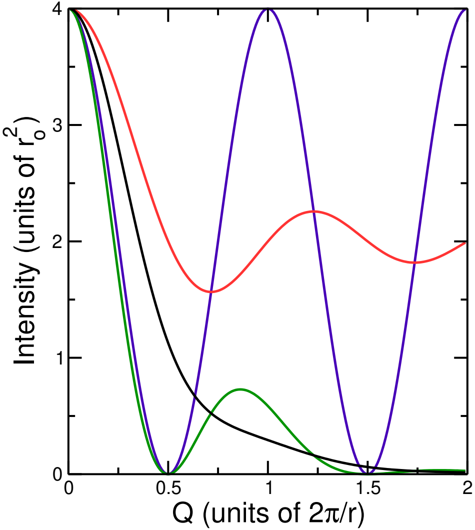

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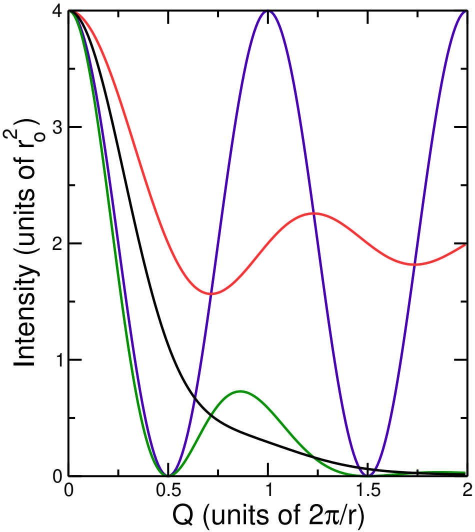

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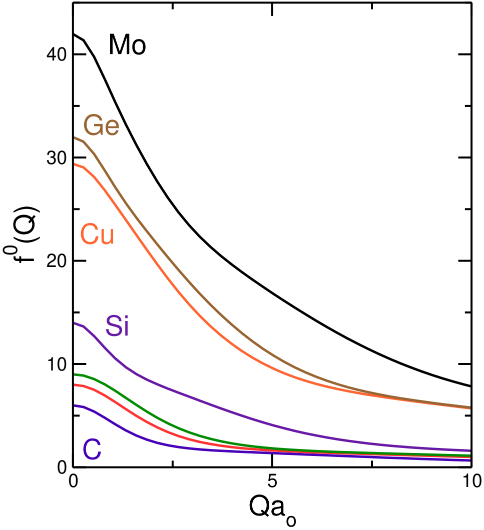

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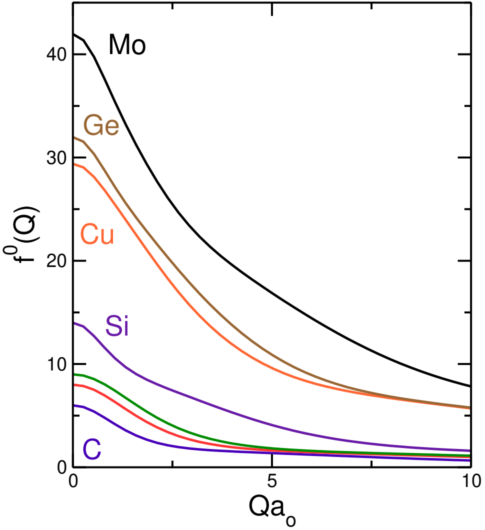

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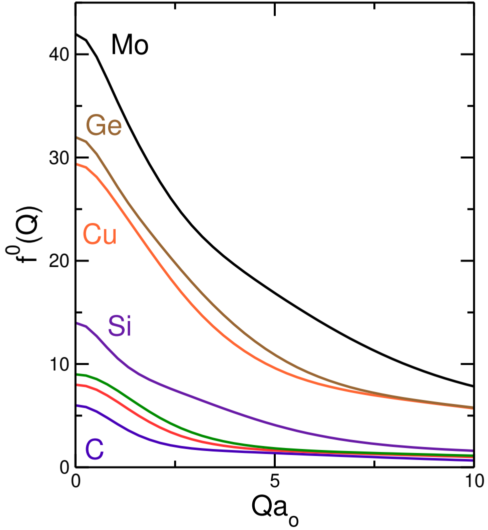

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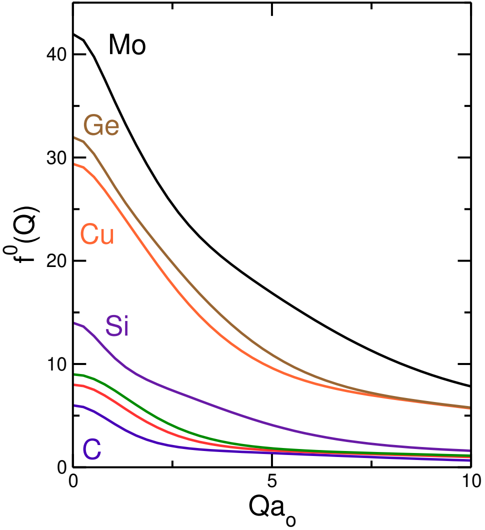

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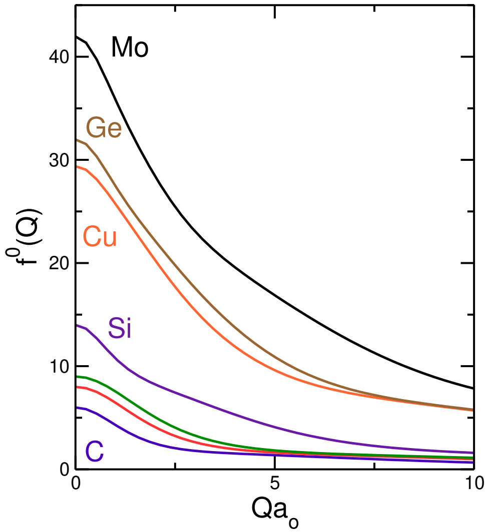

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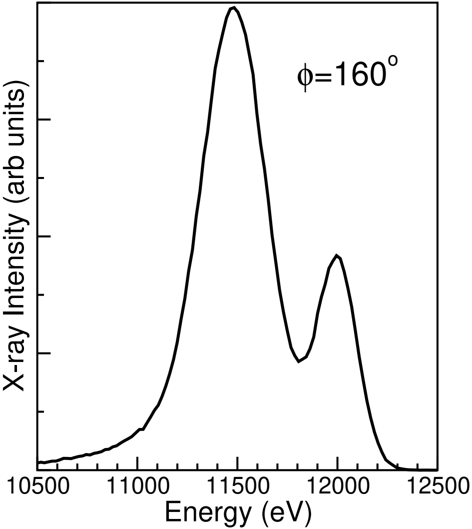

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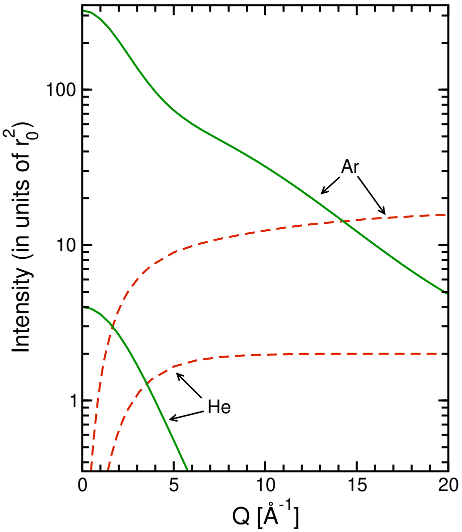

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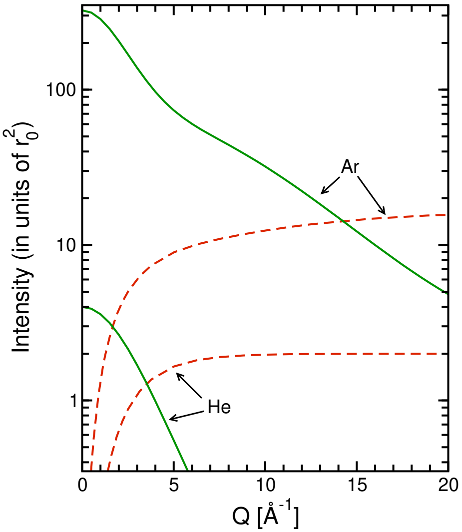

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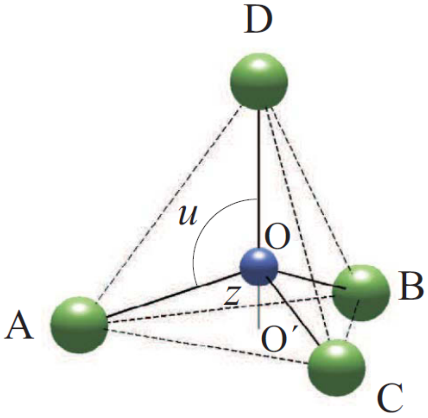

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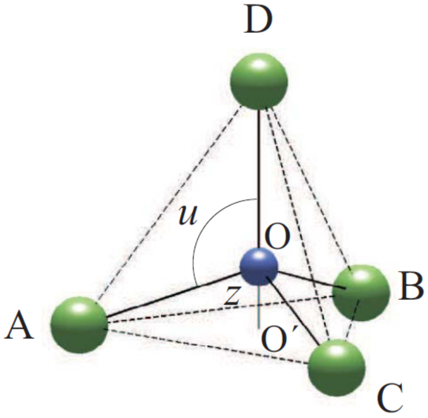

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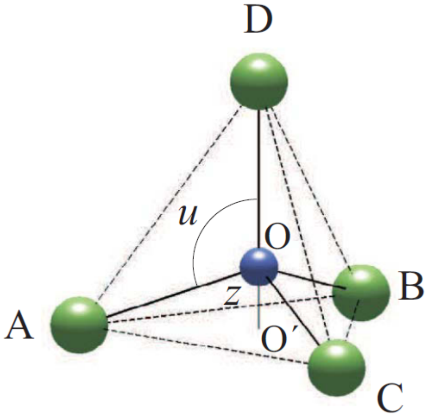

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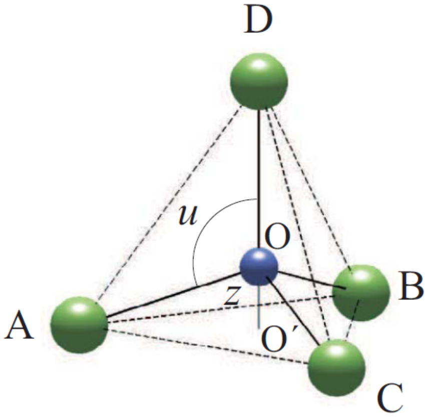

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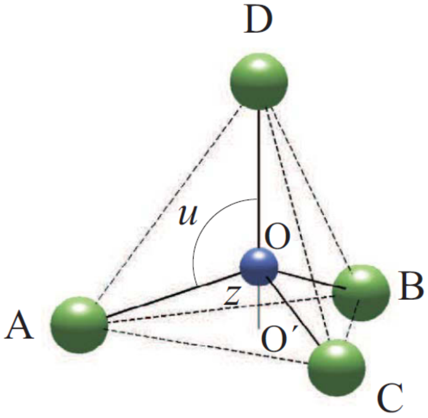

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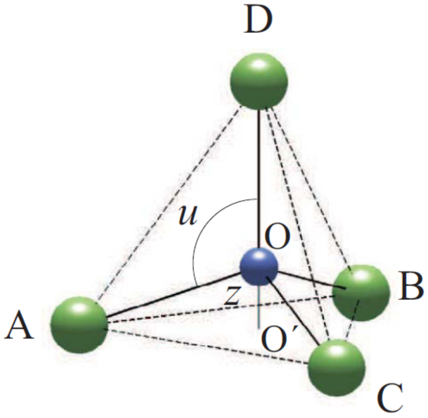

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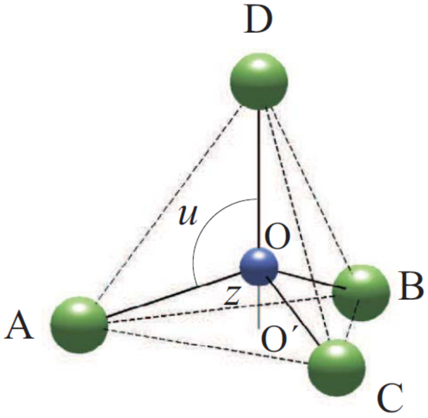

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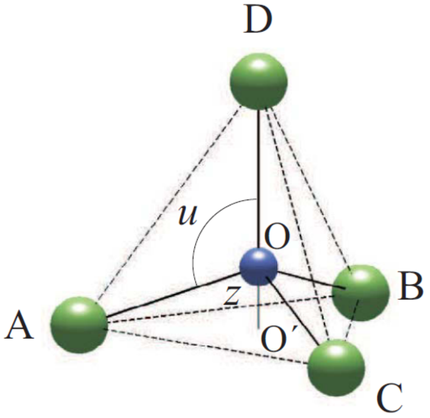

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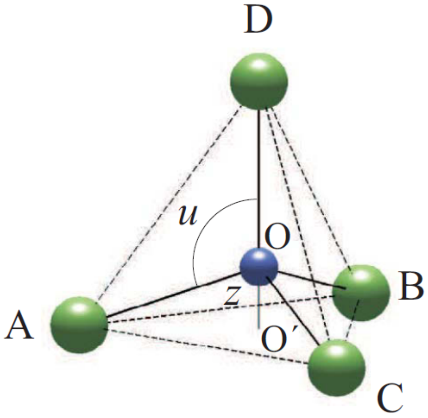

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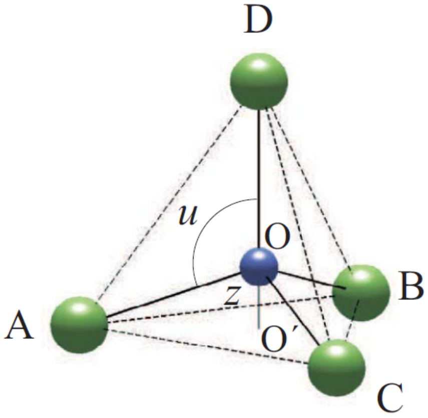

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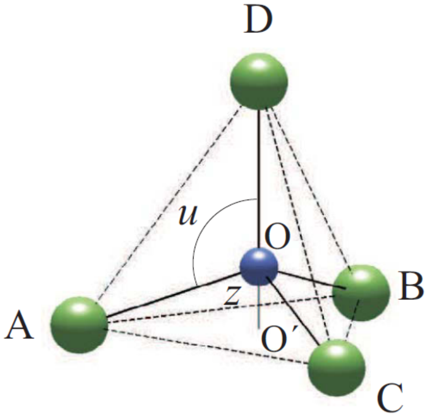

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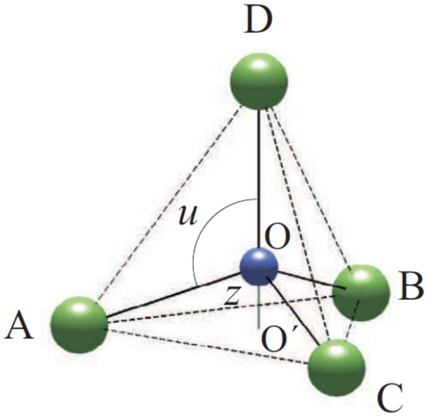

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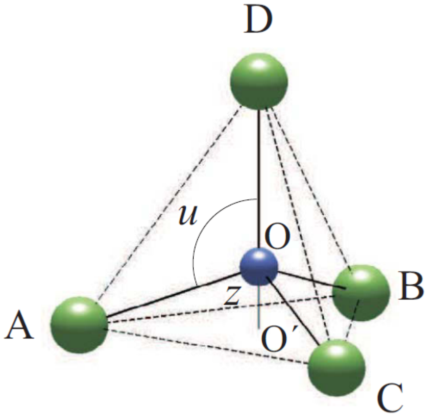

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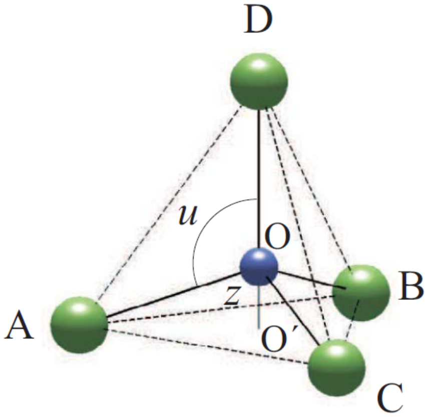

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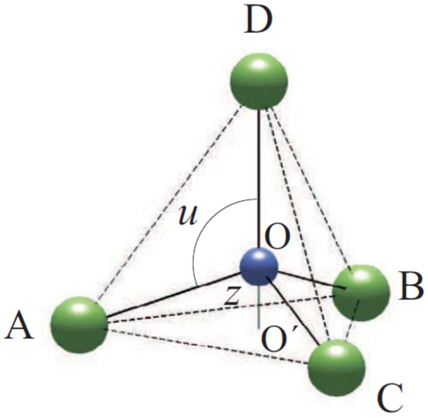

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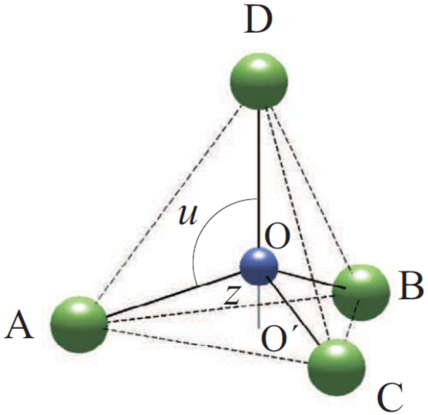

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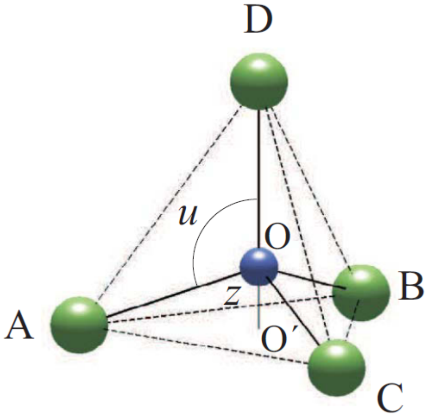

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$$(O'A)^2 = 1 - z^2$$

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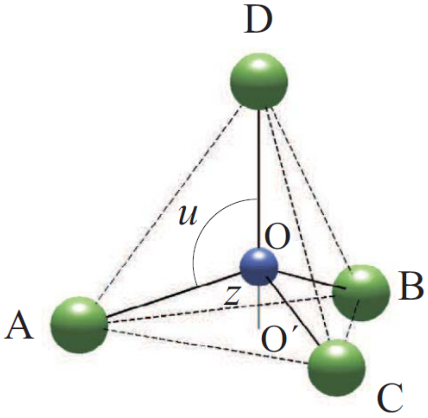

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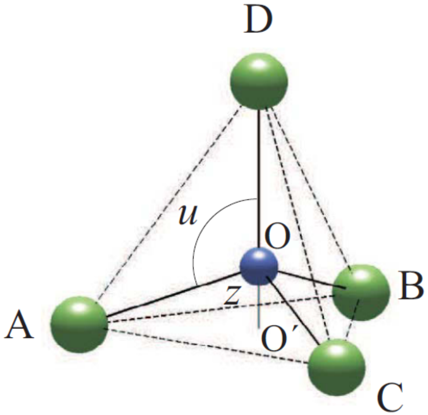

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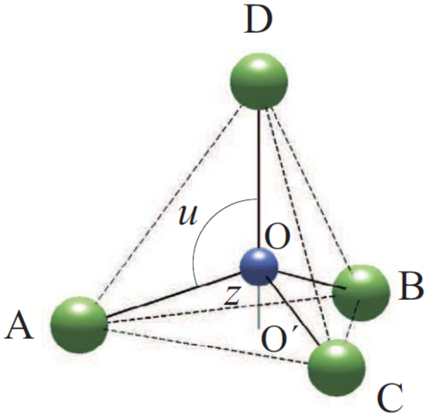

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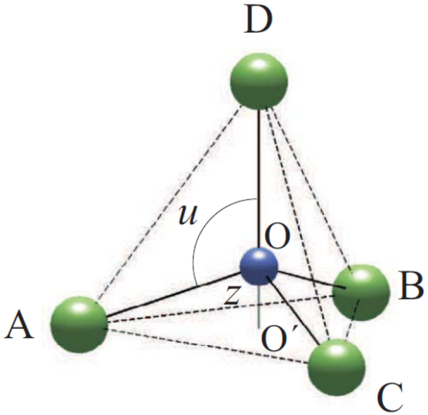

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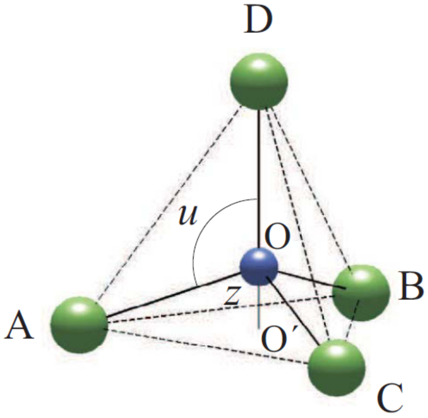

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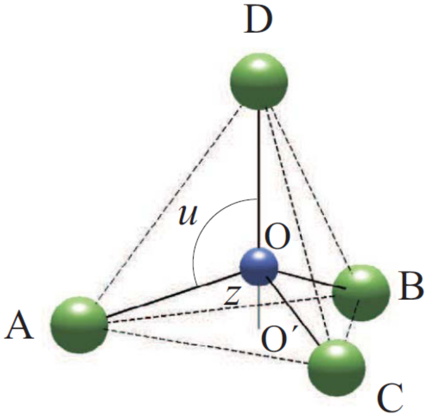

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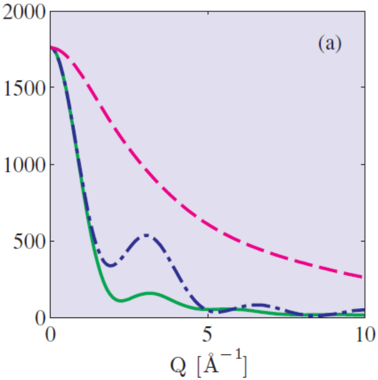

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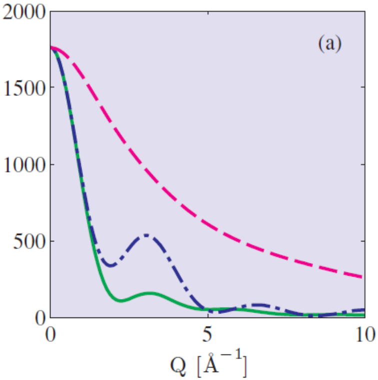

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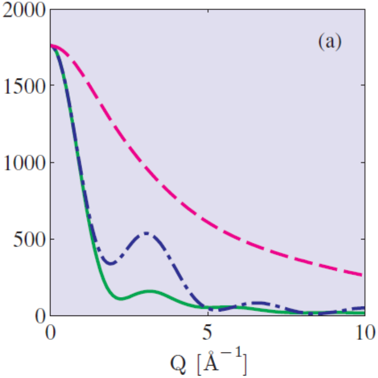

The plot shows the structure factor of CF_4, its orientationally averaged structure factor, and the form factor factor of Mo which has the same number of electrons as CF_4

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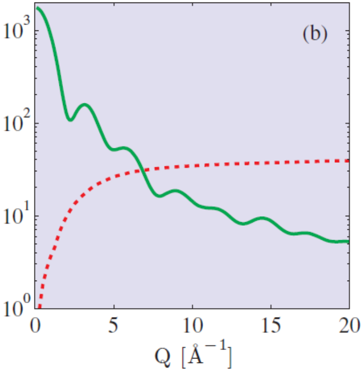

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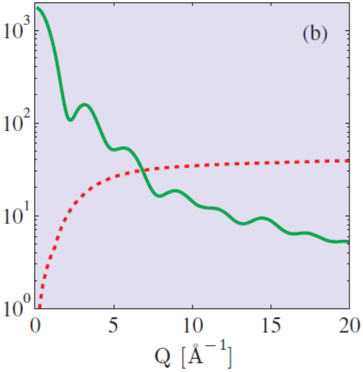


The plot shows the structure factor of CF_4, its orientationally averaged structure factor, and the form factor factor of Mo which has the same number of electrons as CF_4

The logarithmic plot shows the spherically averaged structure factor compared to the inelastic scattering for CF_4

The radial distribution function

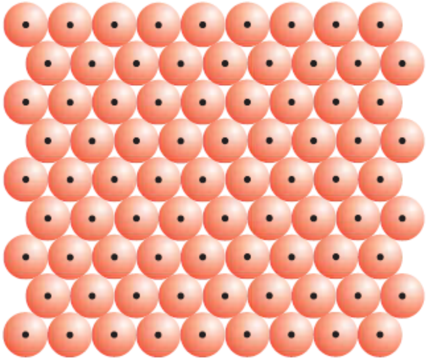
The radial distribution function

Ordered 2D crystal

Amorphous solid or liquid

The radial distribution function

Ordered 2D crystal



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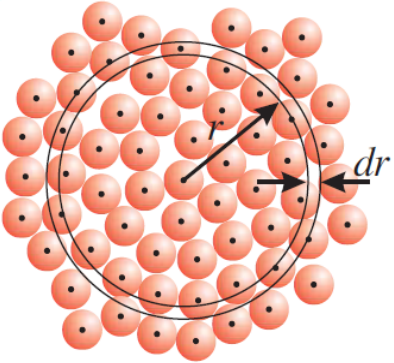

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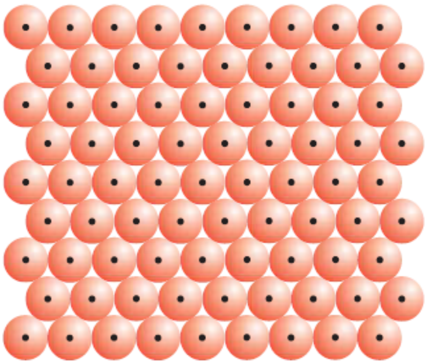

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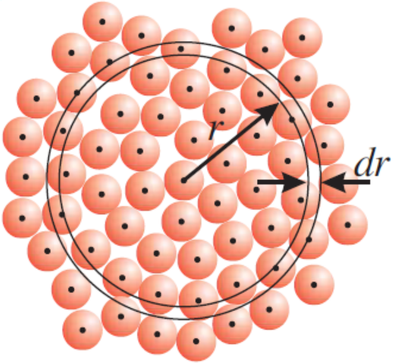

Take a circle (sphere) of radius r and thickness dr and count the number of atom centers lying within the ring.

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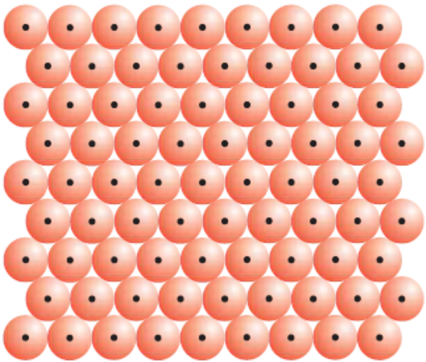
Ordered 2D crystal



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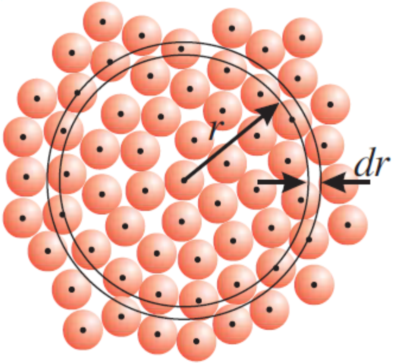

Take a circle (sphere) of radius r and thickness dr and count the number of atom centers lying within the ring. Then expand the ring radius by dr to map out the radial distribution function $g(r)$

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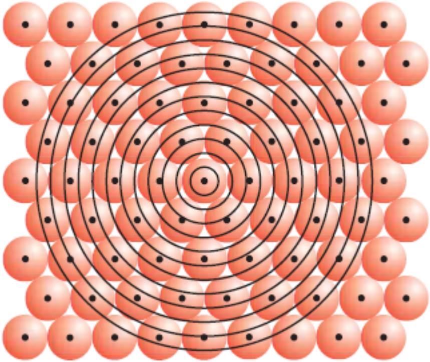
Ordered 2D crystal



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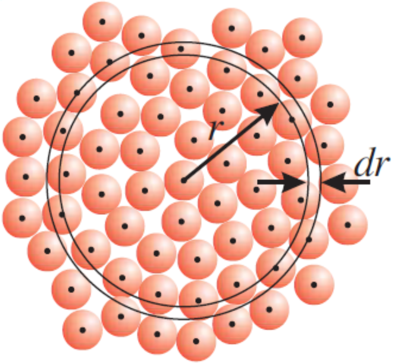

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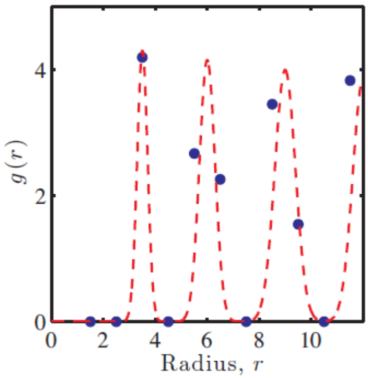

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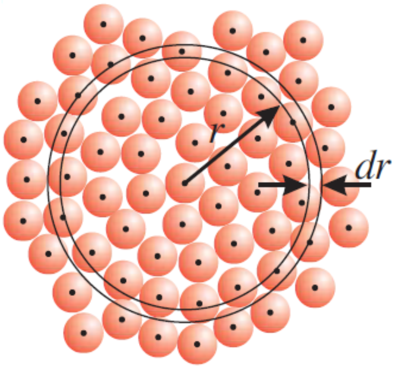

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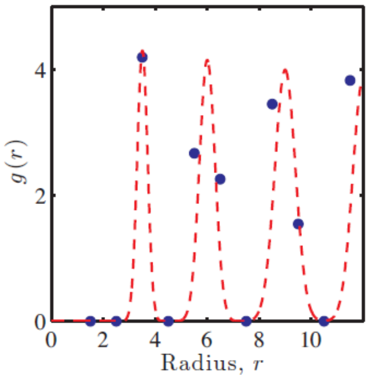

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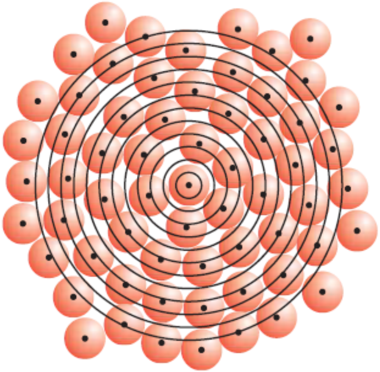

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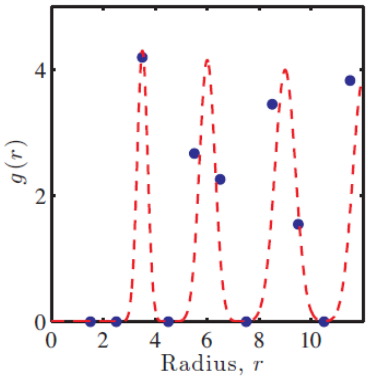

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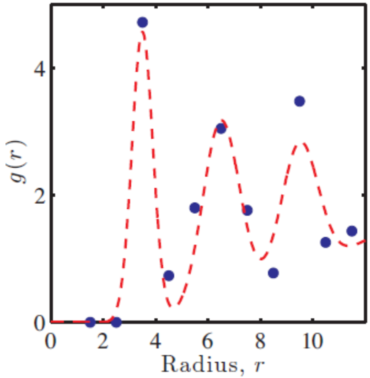

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For the moment, let us ignore the SAXS term and focus on the short range order term.

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Performing an orientational average results in

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For the moment, let us ignore the SAXS term and focus on the short range order term.

$$I^{SRO}(\vec{Q}) = Nf(\vec{Q})^2 + f(\vec{Q})^2 \sum_n \int_V \left[\rho_n(\vec{r}_{nm}) - \rho_{at}\right] e^{i\vec{Q}\cdot(\vec{r}_n - \vec{r}_m)} dV$$

When we average over all choices of origin in the liquid, $\langle \rho_n(\vec{r}_{nm}) \rangle \rightarrow \rho(\vec{r})$ and the sum simplifies to N giving:

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Performing an orientational average results in

$$I^{SRO}(\vec{Q}) = Nf(\vec{Q})^2 + Nf(\vec{Q})^2 \int_0^\infty 4\pi r^2 \left[\rho(r) - \rho_{at}\right] \frac{\sin Qr}{Qr} dr$$

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Which is the sine Fourier Transform of the deviation of the atomic density from its average, $\mathcal{H}(r) = 4\pi r\left[g(r) - 1\right]$

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This formalism holds for both non-crystalline solids and liquids, even though inelastic scattering dominates in the latter.

The relation between radial distribution function and structure factor can be extended to multi-component systems where $g(r) \rightarrow g_{ij}(r)$ and $S(Q) \rightarrow S_{ij}(Q)$.

Structure in supercooled liquid metals

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"Difference in Icosahedral Short-Range Order in Early and Late Transition Metal Liquids," G.W. Lee et al. *Phys. Rev. Lett* **93**, 037802 (2004).

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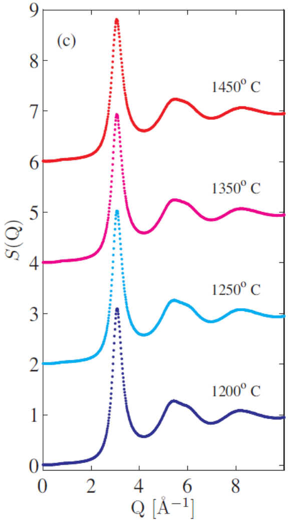

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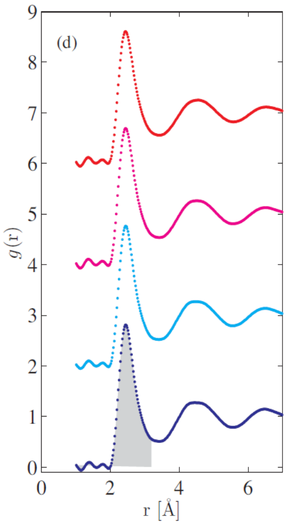

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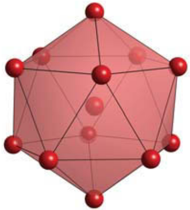
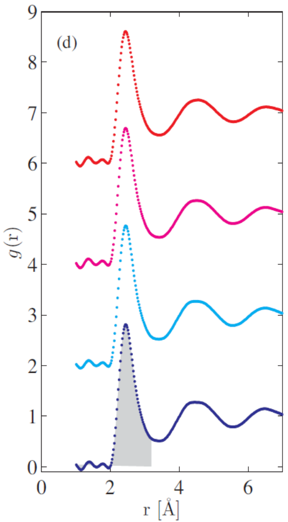


Details in the shape of the oscillations can be indicative of distortions in the icosahedra which depend on the metal species.



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