Today's outline - September 30, 2021

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- Small angle x-ray scattering

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Reading Assignment: Chapter 4.5; Chapter 5.1

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Reading Assignment: Chapter 4.5; Chapter 5.1

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

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- Calculating R_g
- Porod analysis
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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

Liquid scattering review

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

Water dynamics

Liquid scattering can be used to study dynamics

"Seeing real-space dynamics of liquid water through inelastic x-ray scattering," T. Iwashita et al. *Sci. Adv.* **3**, e1603079 (2017).

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In this article, the authors measured the liquid scattering as a function of both momentum, Q, and energy, E, transfer by using analyzers set for a specific energy (21.747 keV) but varying Q and then scanning the incident energy at fixed incident angle

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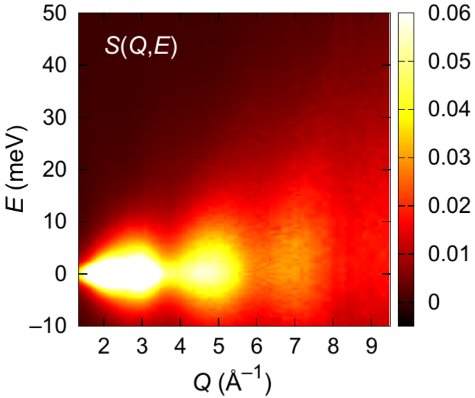

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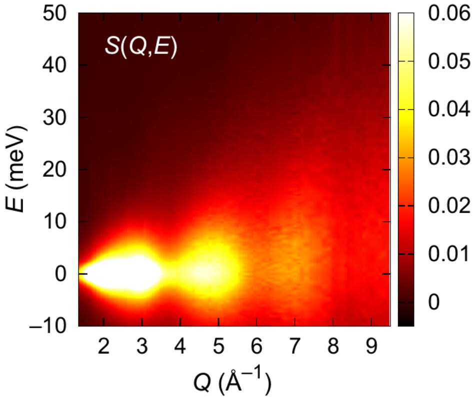

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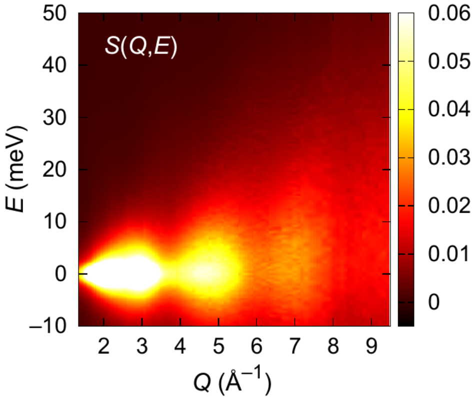

$$g(r,t) - 1 = \frac{1}{2\rho\pi^2 r} \int\int e^{i\omega t} \sin(Qr) QS(Q,E) dQ\, dE$$

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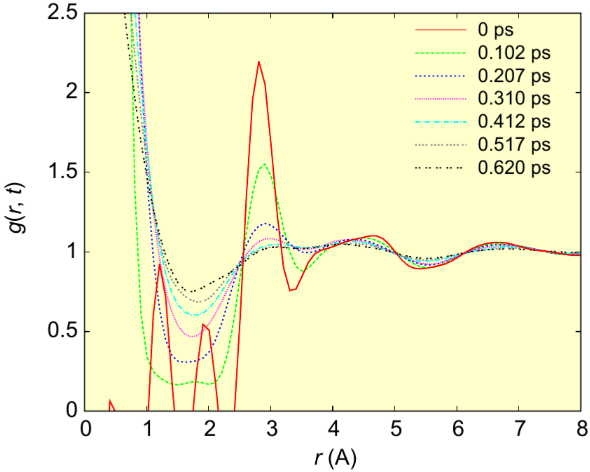

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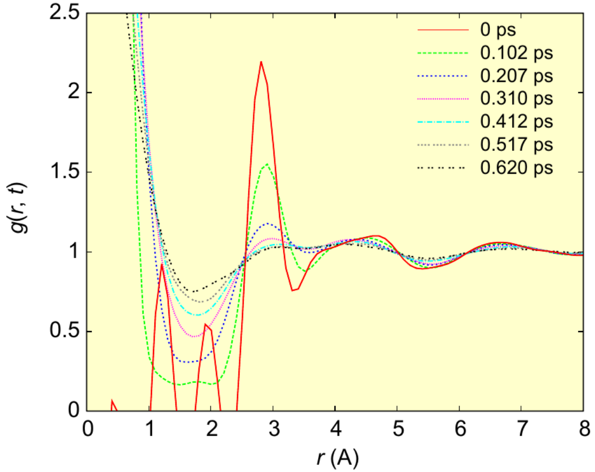

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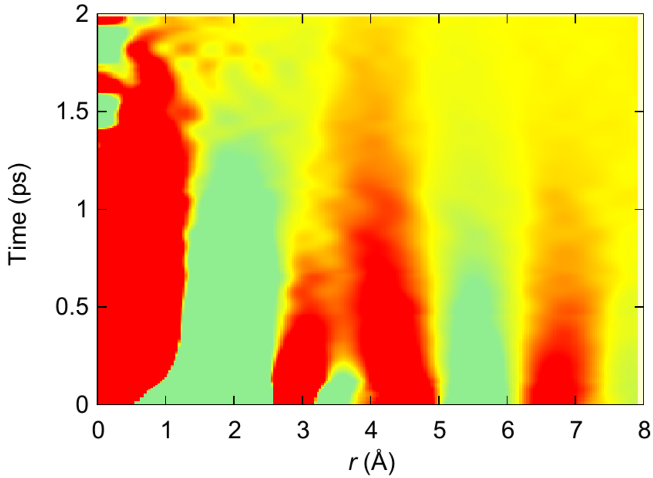

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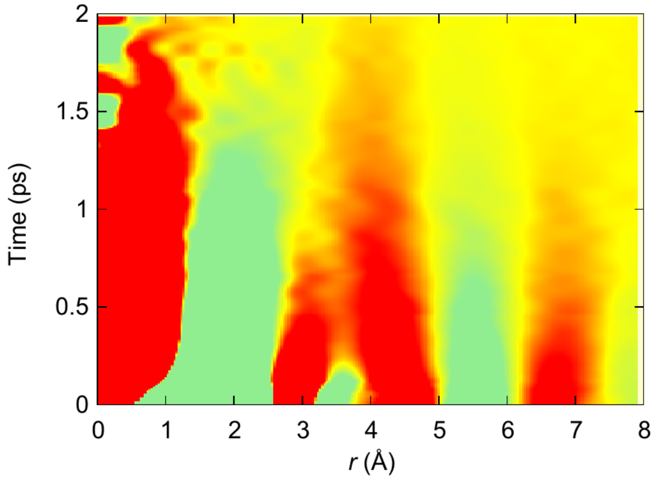

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The first and second peaks are highly coupled in space and time and merge within 0.8 ps. This behavior is different from liquid metals and leads to the viscosity of water.

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Small angle x-ray scattering

$$I(\vec{Q}) = Nf(\vec{Q})^2 + f(\vec{Q})^2 \sum_n \int_V [\rho_n(\vec{r}_{nm}) - \rho_{at}] e^{i\vec{Q}\cdot(\vec{r_n}-\vec{r_m})}\, dV_m + f(\vec{Q})^2 \rho_{at} \sum_n \int_V e^{i\vec{Q}\cdot(\vec{r_n}-\vec{r_m})}\, dV_m$$

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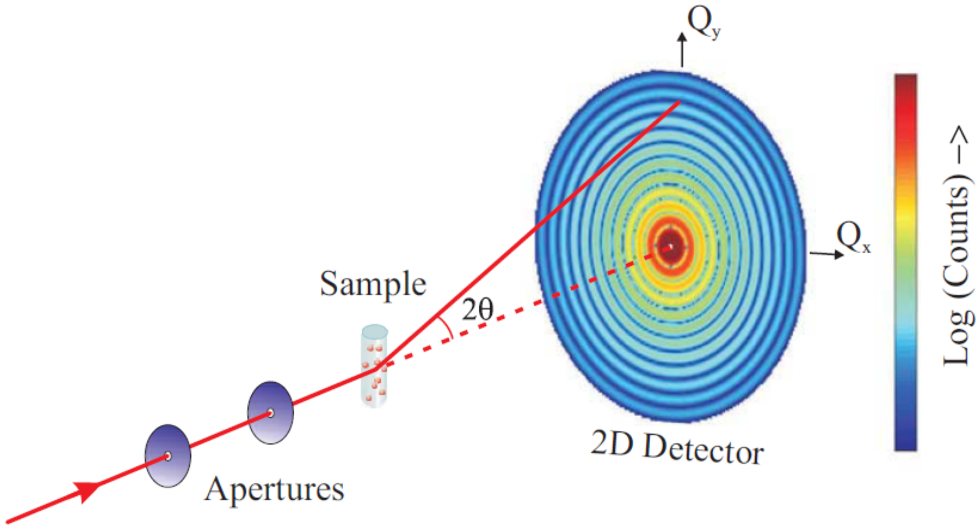
Where we have assumed sufficient averaging and introduced $\rho_{sl} = f\rho_{at}$. This final expression looks just like an atomic form factor but the charge density that we consider here is on a much longer length scale than an atom.

The SAXS experiment



Scattering from a dilute solution

The simplest case is for a dilute solution of non-interacting molecules.

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Where $\Delta\rho = (\rho_{sl,p} - \rho_{sl,0})$, and the form factor depends on the morphology of the particle (size and shape).

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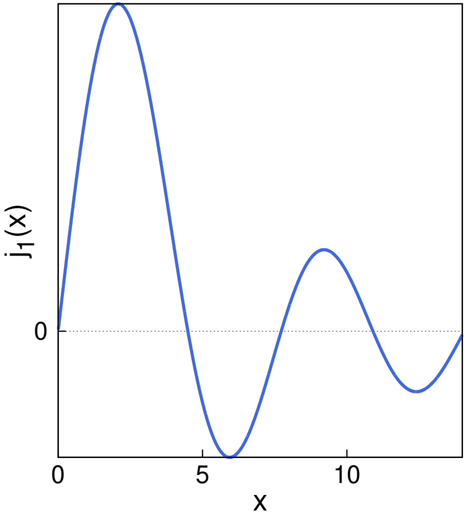

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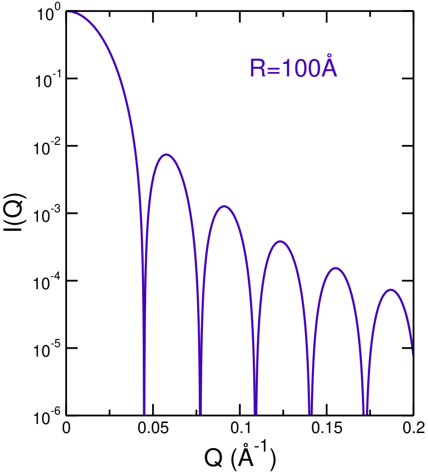

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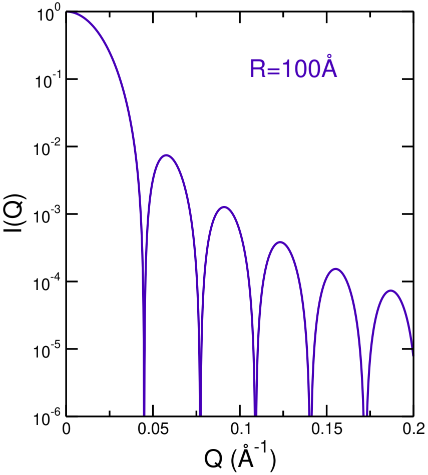

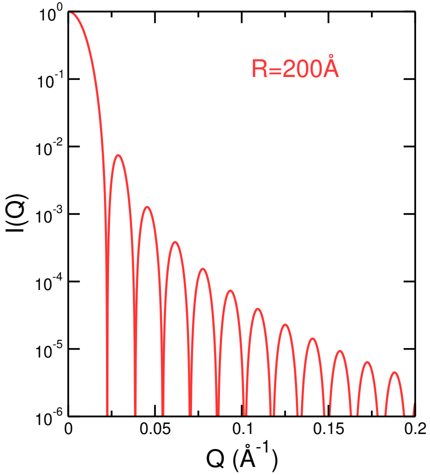

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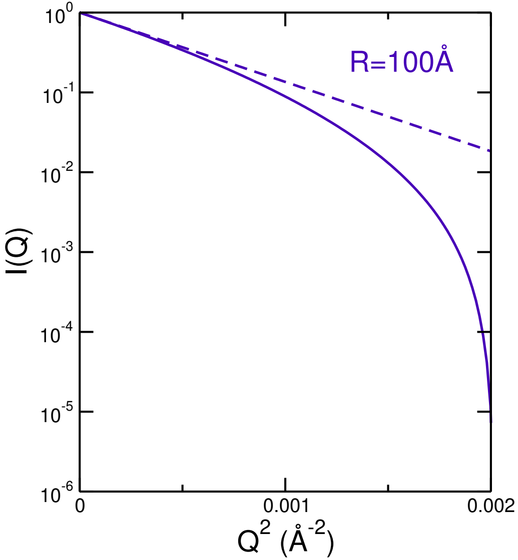

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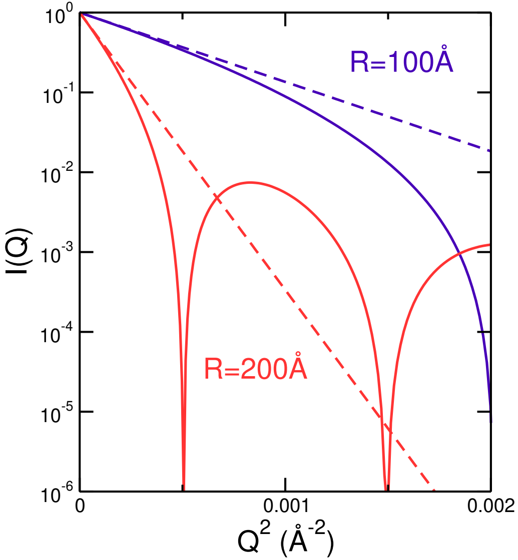

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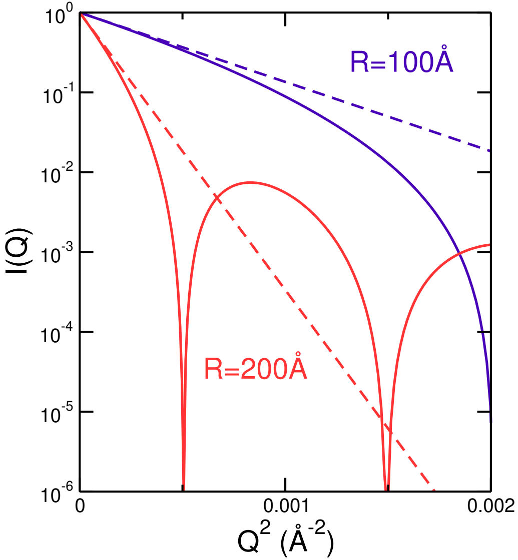

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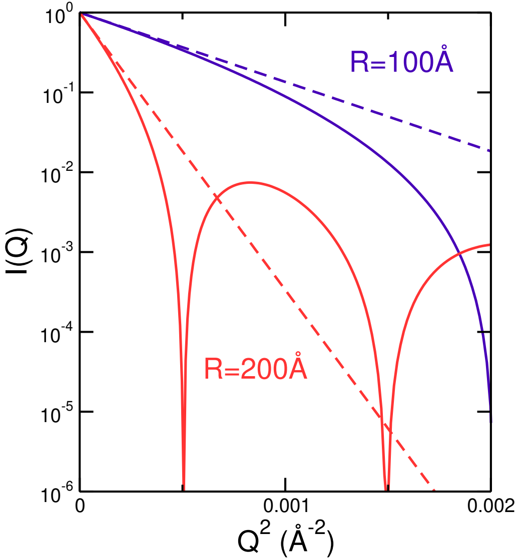

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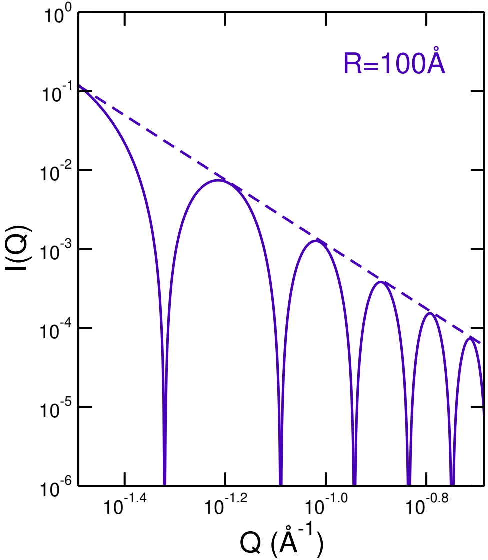

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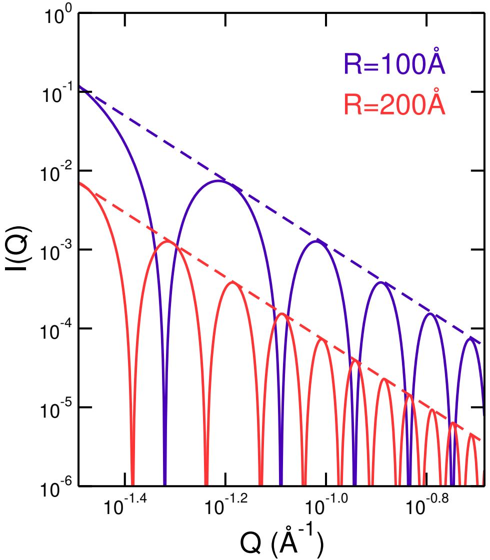

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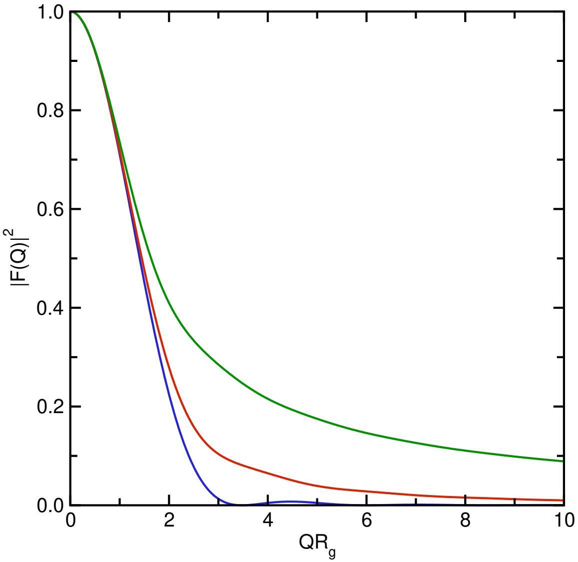

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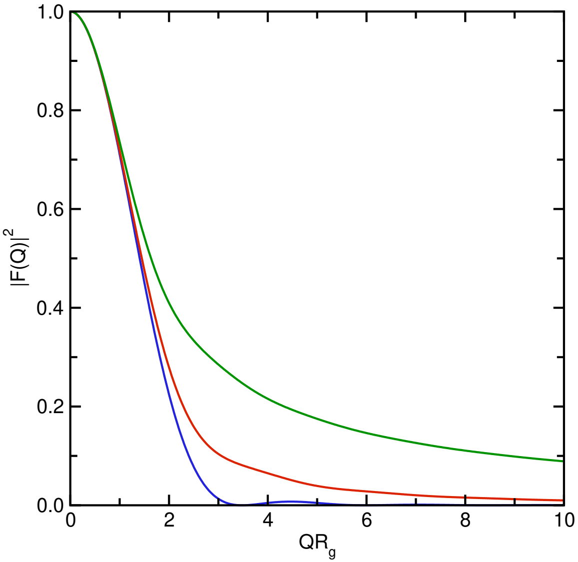

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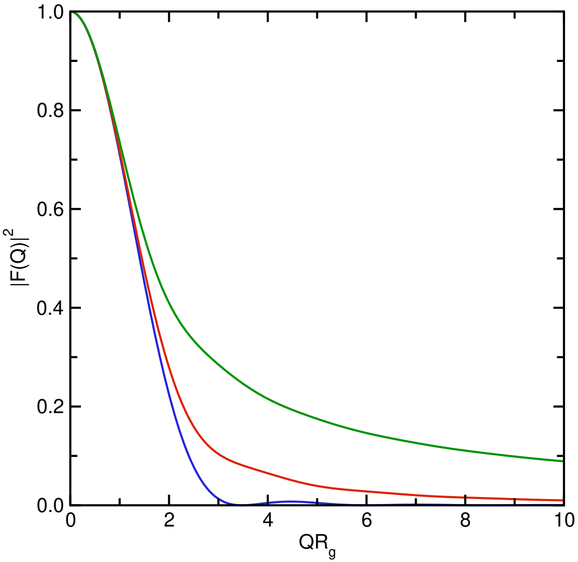

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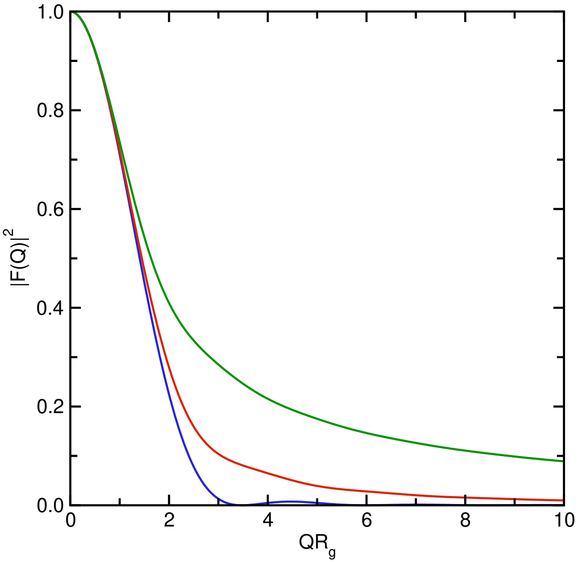

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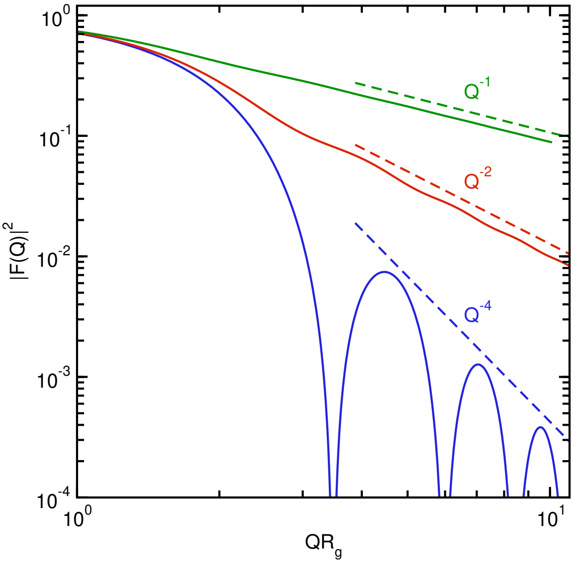

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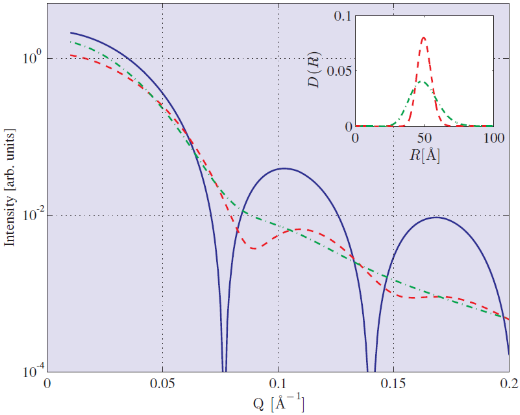

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The sum is over structural levels starting with the smallest. For each level there is a Guinier exponential prefactor (G_i), a radius of gyration ($R_{g,i}$), a power law constant prefactor (B_i), and a power law exponent (P_i).

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It is important not to include more levels than are significant physically