Methoden moderner Röntgenphysik: Streuung und Abbildung

Lecture 7	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2019		
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Location	Lecture hall AP, Physics, Jungiusstraße		
Date	Tuesdays	12:30 - 14:00	(starting 2.4.)
	Thursdays	8:30 - 10:00	(until 11.7.)

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Part I:

Basics of X-ray Physics

by Gerhard Grübel (GG)

Introduction
Overview, Introduction to X-ray Scattering

X-ray Scattering Primer
Elements of X-ray Scattering

Sources of X-rays, Synchrotron Radiation
Laboratory Sources, Accelerator Bases Sources

Reflection and Refraction from Interfaces
Snell's Law, Fresnel Equations

Kinematical Diffraction (I)
Diffraction from an Atom, a Molecule, from Liquids, Glasses, …

Kinematical Diffraction (II)
Diffraction from a Crystal, Reciprocal Lattice, Structure Factor, …

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Small Angle Scattering, and Soft Matter
Introduction, Form Factor, Structure Factor, Applications, ...

Anomalous Diffraction
Introduction into Anomalous Scattering, ...

Introduction into Coherence
Concept, First Order Coherence, ...

Coherent Scattering
Spatial Coherence, Second Order Coherence, ...

Applications of Coherent Scattering
Imaging and Correlation Spectroscopy, ...

Small Angle X-ray Scattering (SAXS)

From Eq. (**)

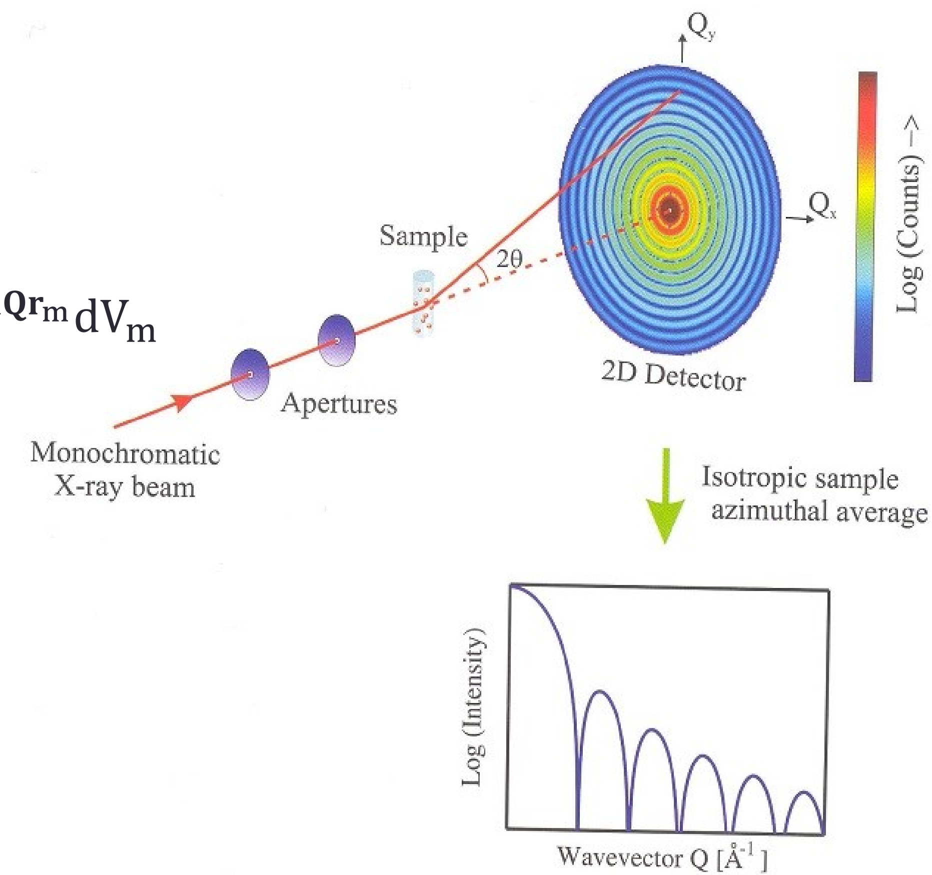
$$I_{SAXS}(Q) = f^2 \sum_n \int_V \rho_{at}\, e^{iQ(r_n - r_m)} dV_m$$

$$= f^2 \sum_n e^{iQr_n} \int_V \rho_{at}\, e^{-iQr_m} dV_m$$

$$= f^2 \int_V \rho_{at}\, e^{iQr_n} dV_n \int_V \rho_{at}\, e^{-iQr_m} dV_m$$

$$\Rightarrow I_{SAXS}(Q) = \left| \int_V \rho_{sl}\, e^{iQr} dV \right|^2$$

with $\rho_{sl} = f\,\rho_{at}$



SAXS (Form Factor)

The form factor of isolated particles

$$I_{SAXS}(Q) = (\rho_{sI,p} - \rho_{sI,0})^2 \left| \int_V e^{iQr} dV_p \right|^2$$

Where $\rho_{sl,p}$, $\rho_{sl,0}$ are the scattering length densities of the particle (p) and solvent (0) and V_p is the volume of the particle.

Using the particle form factor $$F(Q) = \frac{1}{V_p} \int_{V_p} e^{iQr} dV_p$$

one finds $I_{SAXS}(Q) = \Delta\rho 2\ V^2{}_p\ |F(Q)|2$ with $\Delta\rho = \rho_{sI,p} - \rho_{sI,0}$

The form factor depends on the morphology (size and shape of the particles) and can be evaluated analytically only in a few cases:

For a sphere with radius R one finds:

$$F(Q) = \frac{1}{V_p} \int_0^R \int_0^{2\pi} \int_0^{\pi} e^{iQr\cos(\theta)} r^2 \sin\theta\, d\theta d\phi dr = \frac{1}{V_p} \int_0^R 4\pi \frac{\sin(Qr)}{Qr} r^2 dr$$

$$= 3\frac{\sin(QR) - Qr\cos(QR)}{(QR)^3} = 3\frac{J_1(QR)}{QR}$$

with $J_1(x)$: Bessel function of the first kind.

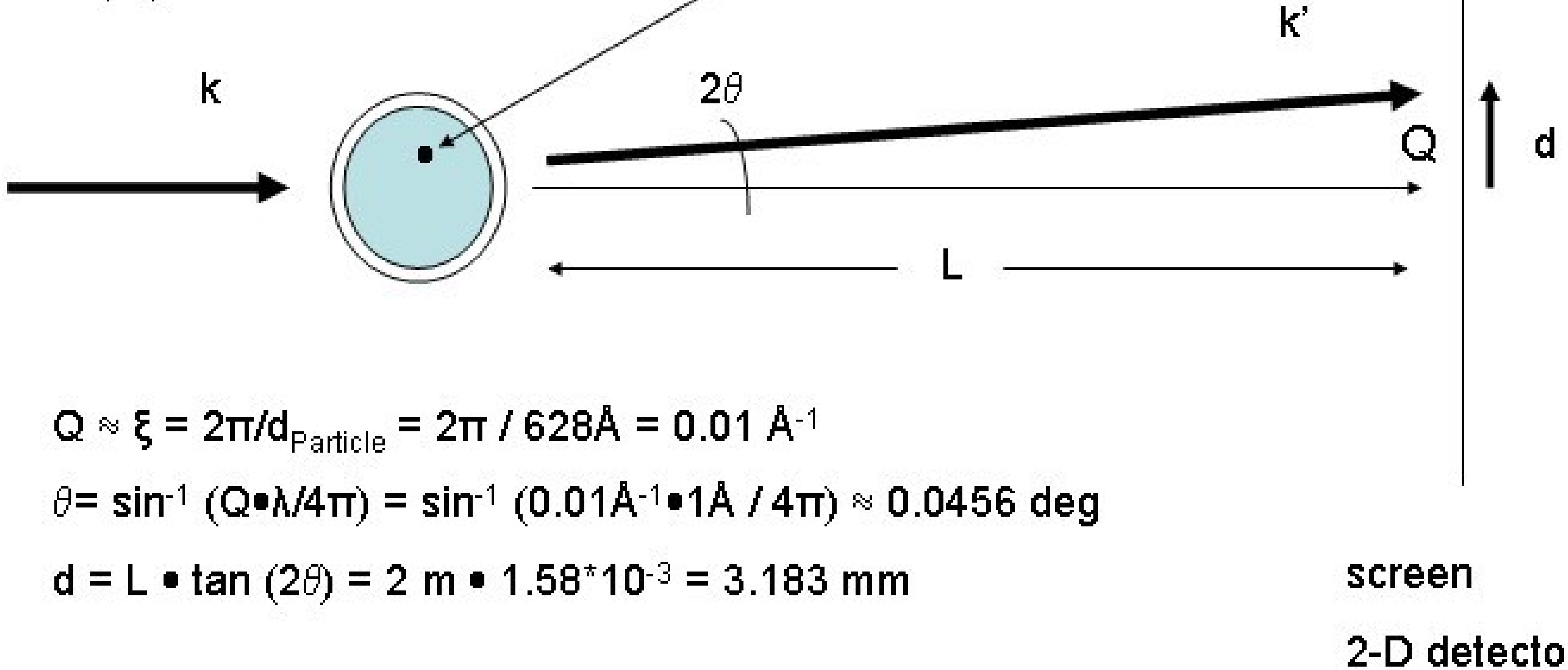
For Q→0: $|F(Q)|^2 = 1$ and $I_{SAXS}(Q) = = \Delta\rho^2 V^2{}_p$

Experimental Set-up (SAXS)

Consider objects (nano-structures) of sub-μm size

$\sin\theta = (Q/2) / k = (Q\bullet\lambda)/ 4\pi$

$\tan(2\theta) = d / L$



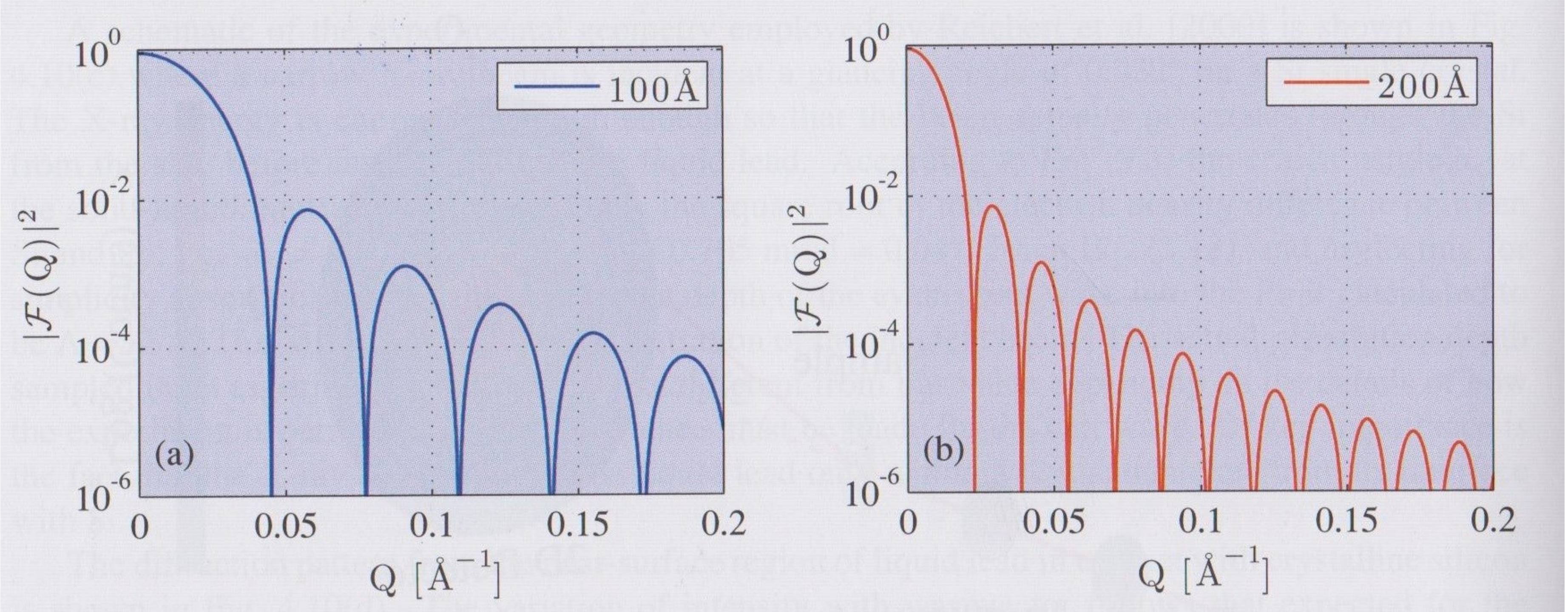
$Q \approx \xi = 2\pi/d_{Particle} = 2\pi / 628Å = 0.01\ Å^{-1}$

$\theta = \sin^{-1}(Q\bullet\lambda/4\pi) = \sin^{-1}(0.01Å^{-1}\bullet 1Å / 4\pi) \approx 0.0456$ deg

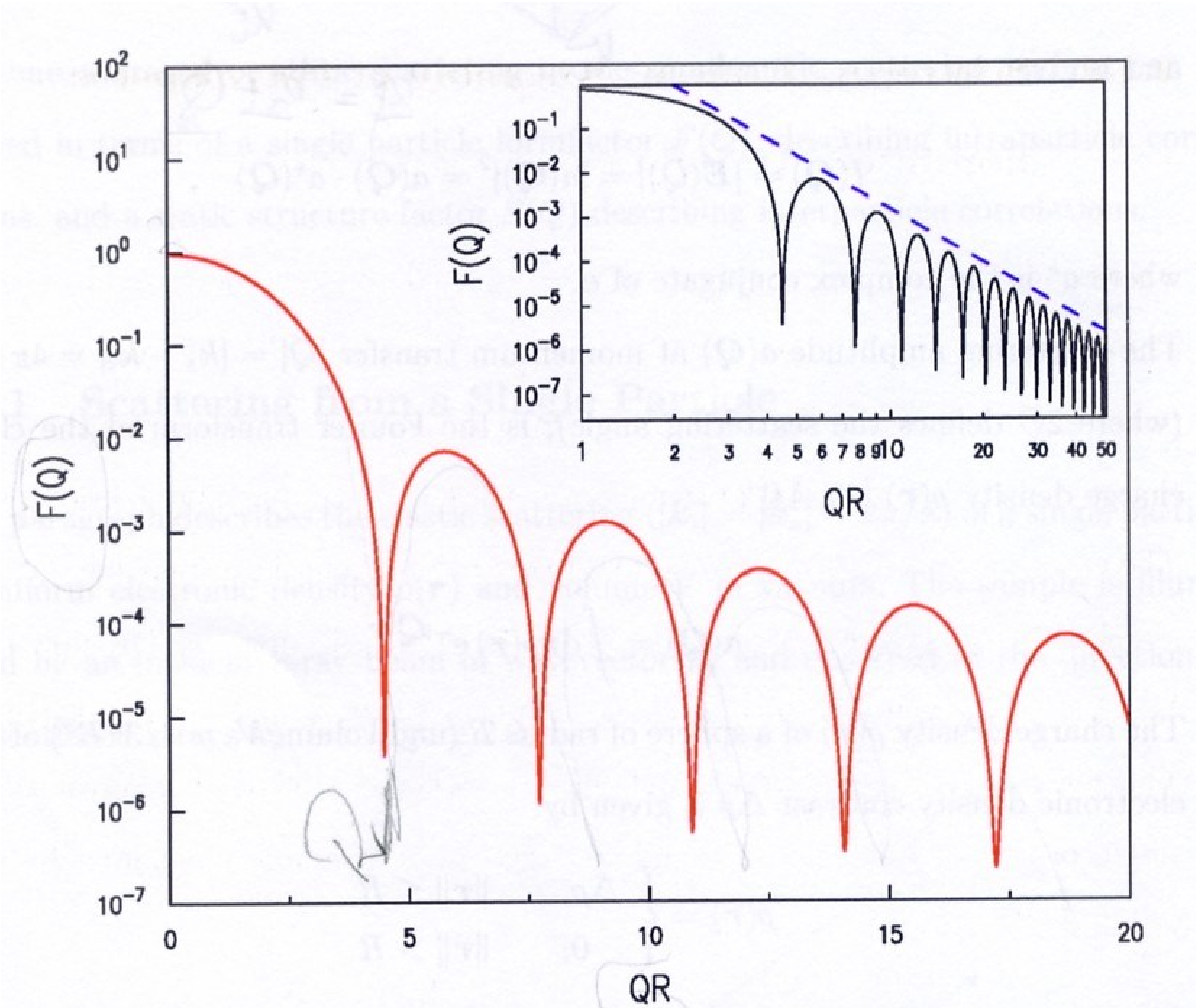
$d = L \bullet \tan(2\theta) = 2\ m \bullet 1.58{*}10^{-3} = 3.183$ mm

Form Factor for Monodisperse Spheres

Monodisperse spheres of radius 10nm and 20 nm



Form Factor for Monodisperse Spheres



The Small Q Limit: Guinier Regime

For $QR \rightarrow 0$:

$$F(Q) \approx \frac{3}{(QR)^3}\left[QR - \frac{(QR)^3}{6} + \frac{(QR)^5}{120} = \cdots - QR\left(1 - \frac{(QR)^2}{2} + \frac{(QR)4}{24}\right)\right]$$

$$\approx 1 - \frac{(QR)^2}{10}$$

Thus:

$$I_{SAXS}(Q) \approx \Delta\rho^2 V^2{}_p \left[1 - \frac{(QR)^2}{10}\right]^2 \approx \Delta\rho^2 V^2{}_p \left[1 - \frac{(QR)^2}{5}\right]$$

Thus the QR → 0 limit can be used to determine the particle radius R via:

$$I_{SAXS}(Q) \approx \Delta\rho 2\, V^2{}_p\, e^{-\frac{(QR)^2}{5}} \qquad QR << 1 \qquad [e^{-x} = 1 - x]$$

Thus: plotting ln $[I_{SAXS}(Q)]$ vs. Q^2 reveals a slope ~ $R^2/5$ $\Rightarrow$ R

The Large Q Limit: Porod Regime

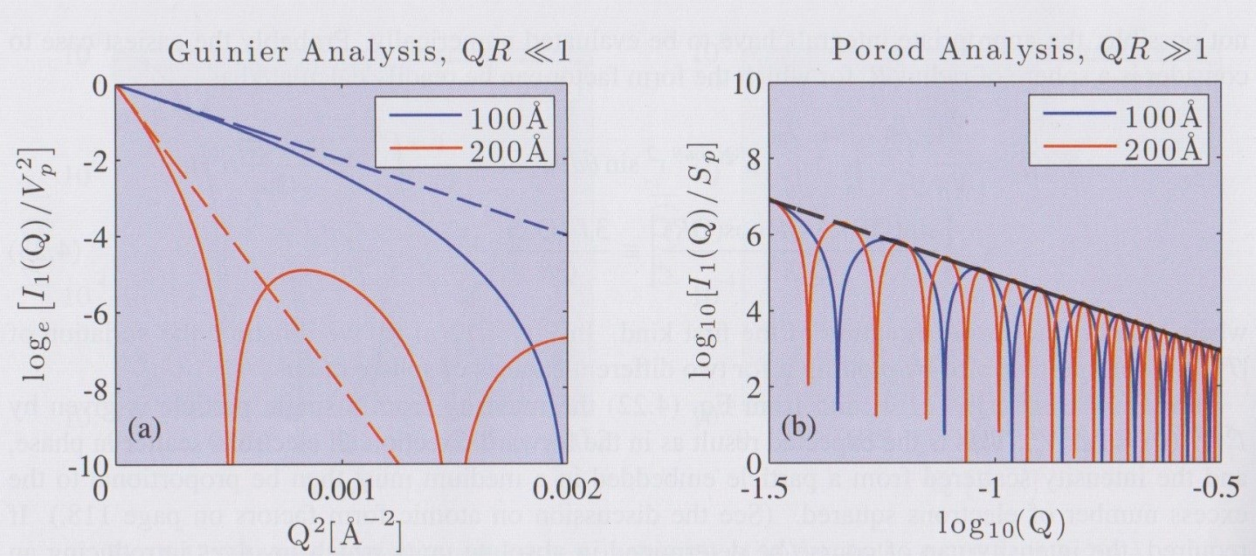
For QR >> 1: wavelength small compared to particle size

$$F(Q) = 3\left[\frac{\sin(QR)}{(QR)^3} - \frac{\cos(QR)}{(QR)^2}\right] \approx 3\left[-\frac{\cos(QR)}{(QR)^2}\right]$$

When QR >> 1 $\cos^2(x)$ oscillates towards ½ and

$$I_{SAXS(Q)} = 9\Delta\rho^2 V^2{}_p \frac{<\cos^2(QR)>}{(QR)4} = \frac{9\Delta\rho^2 V_p^2}{2(QR)^4}$$

Thus: $I_{SAXS}(Q) \sim \frac{1}{Q^4}$



Radius of Gyration

Radius of gyration: root mean sqare distance from the particle’s center

$$R_G = \frac{1}{V_p}\int_{v_p} r^2 dV_p$$

$$R_G^2 = \frac{\int_{v_p} dV_p \, \rho_{sI,p}(r) r^2 dV_p}{\int_{v_p} \rho_{sI,p}(r) dV_p}$$

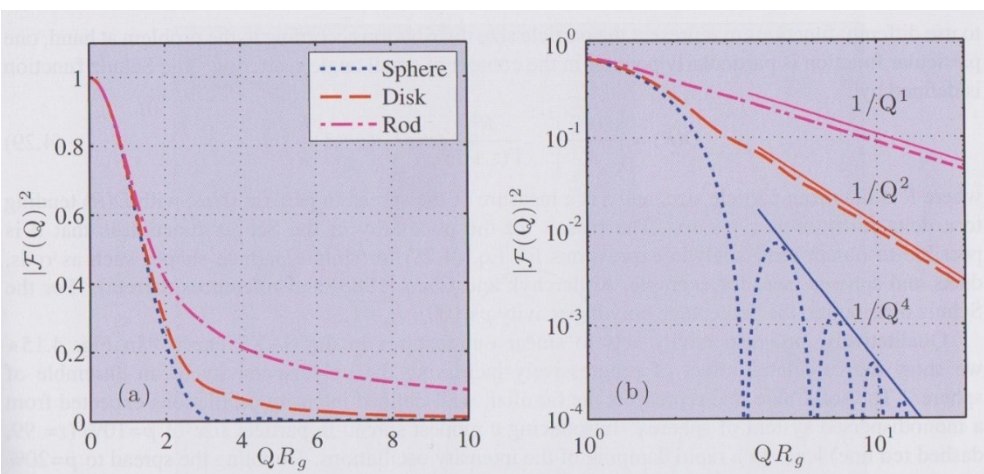
For uniform spheres: $R^2{}_G = {}^3/{}_5 R^2$

$$I^{SAXS}(Q) \approx \Delta\rho^2 V_P^2 \, e^{(-QR_G)^2/3}$$

Form Factor and Particle Shape

$$F(Q) = \frac{1}{V_p} \int_{V_p} e^{iQr} dV_p$$

	$\|F(Q)\|^2$	RG	Porod Exp
Sphere (d=3)	$\left(\frac{3J_1(QR)}{QR}\right)^2$	$\sqrt{\frac{3}{5}}$ R	-4
Disc (d=3)	$\frac{2}{(QR)^2}\left(1 - \frac{J_1(2QR)}{QR}\right)$	$\sqrt{\frac{1}{2}}$ R	-2
Rod (d=1)	$\frac{2Si(QL)}{QL} - \frac{4\sin^2(QR/2)}{(QL)^2}$	$\sqrt{\frac{1}{12}}$ L	-1



with: Si(x) $_0\int^x$ sint/t dt

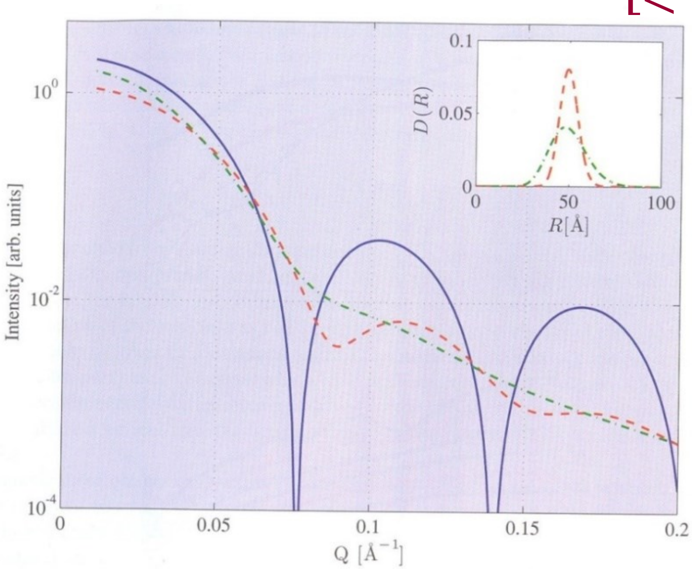
Polydispersity

Realistic ensembles of particles display a certain distribution of particle sizes that shall be disribed by a distribtion function D(R). Thus the scattering intensity may be written as

$$I_{SAXS}(Q) = \Delta\rho 2\ 0\int\infty\ D(R)\ V^2{}_p\ |F(Q,R)|2\ dR$$

with ${}_0\int^\infty D(R)\,dR = 1.$ A frequently used distribution function is the so-called Schultz function, where z is a measure of the polydispersity:

$$D(R) = \left[\frac{z+1}{<R>}\right]^{z+1} \frac{R^z}{\Gamma(z+1)} e^{\left(-(z+1)\frac{R}{<R>}\right)}$$



Structure Factor

Interparticle interactions:

S(Q): structure factor

$$I_{SAXS}(Q) = \Delta\rho 2\, V^2_p \; |F(Q)|^2 \; S(Q)$$

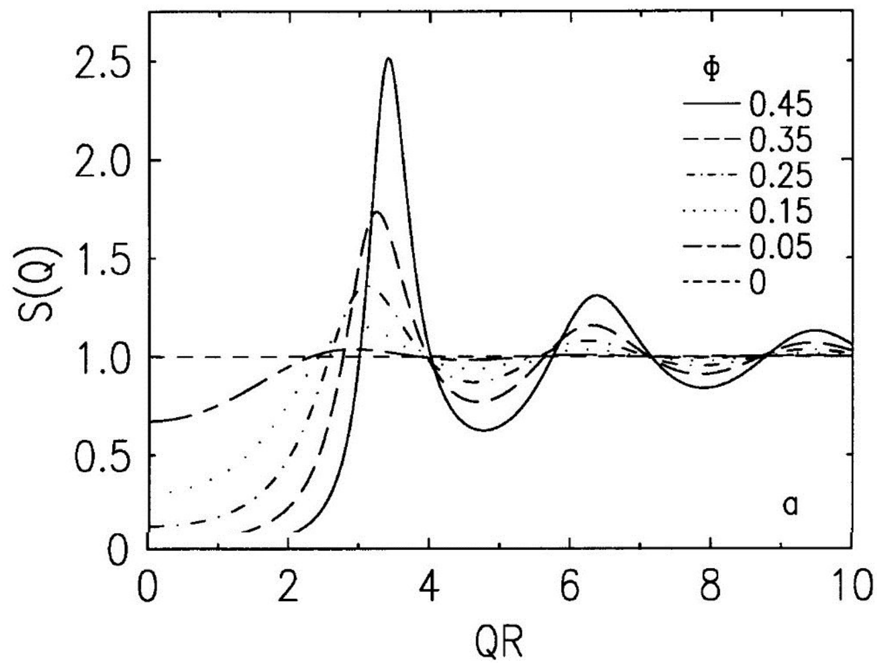
$$S(Q) = \frac{1}{nN} < \sum^{N}_{i,j} \; e^{i\mathbf{Q}(R_i - R_j)} >$$

$$= \int d^3r \, e^{iQr} \bullet g(r)$$

<u>Hard sphere structure factor:</u>

$$V(r) = 0 \quad \text{for } r \geq d$$

$$V(r) = \infty \quad \text{for } r < d$$



SAXS Experiment

- measure I(Q)
- model F(Q)
- for spherical particles I(Q)=F(Q)•S(Q)
- get and model S(Q)