

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecture 7	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2017 G. Grübel, A. Philippi-Kobs, O. Seeck, T. Schneider, L. Frenzel, M. Martins, W. Wurth		
Location	Lecture hall AP, Physics, Jungiusstraße		
Date	Tuesday	12:30 - 14:00	(starting 4.4.)
	Thursday	8:30 - 10:00	(until 13.7.)



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, ...



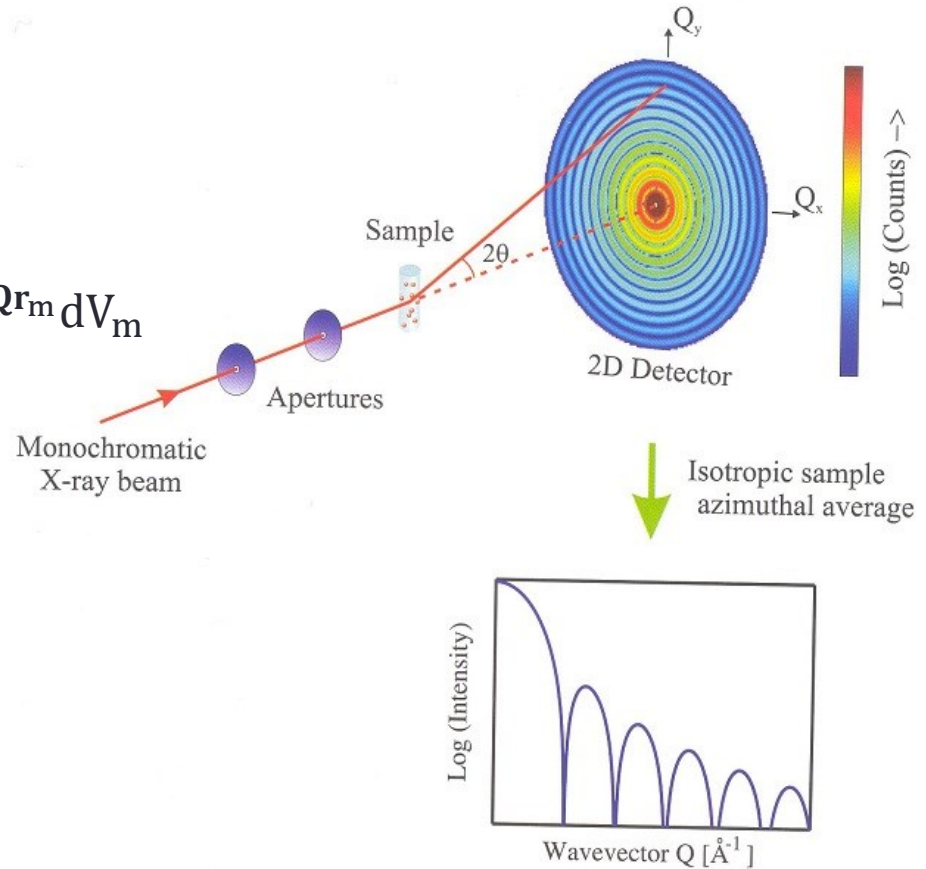
Small Angle X-ray Scattering (SAXS)

From Eq. (**)

$$\begin{aligned}
 I_{\text{SAXS}}(\mathbf{Q}) &= f^2 \sum_n \int_v \rho_{\text{at}} e^{i\mathbf{Q}(\mathbf{r}_n - \mathbf{r}_m)} dV_m \\
 &= f^2 \sum_n e^{i\mathbf{Q}\mathbf{r}_n} \int_v \rho_{\text{at}} e^{-i\mathbf{Q}\mathbf{r}_m} dV_m \\
 &= f^2 \int_v \rho_{\text{at}} e^{i\mathbf{Q}\mathbf{r}_n} dV_n \int_v \rho_{\text{at}} e^{-i\mathbf{Q}\mathbf{r}_m} dV_m
 \end{aligned}$$

$$\Rightarrow I_{\text{SAXS}}(\mathbf{Q}) = \left| \int_v \rho_{\text{sl}} e^{i\mathbf{Q}\mathbf{r}} dV \right|^2$$

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



SAXS (Form Factor)

The form factor of isolated particles

$$I_{\text{SAXS}}(Q) = (\rho_{\text{sl,p}} - \rho_{\text{sl,0}})^2 \left| \int_{V_p} e^{iQr} dV_p \right|^2$$

Where $\rho_{\text{sl,p}}$, $\rho_{\text{sl,0}}$ 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 $I_{\text{SAXS}}(Q) = \Delta\rho^2 V_p^2 |F(Q)|^2$ with $\Delta\rho = \rho_{\text{sl,p}} - \rho_{\text{sl,0}}$

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:

$$\begin{aligned}
 F(Q) &= \frac{1}{V_p} \int_0^R \int_0^{2\pi} \int_0^\pi e^{iQr \cos(\theta)} r^2 \sin\theta \, d\theta d\phi dr = \frac{1}{V_p} \int_0^R 4\pi \frac{\sin(Qr)}{Qr} r^2 dr \\
 &= 3 \frac{\sin(QR) - QR \cos(QR)}{(QR)^3} = 3 \frac{J_1(QR)}{QR}
 \end{aligned}$$

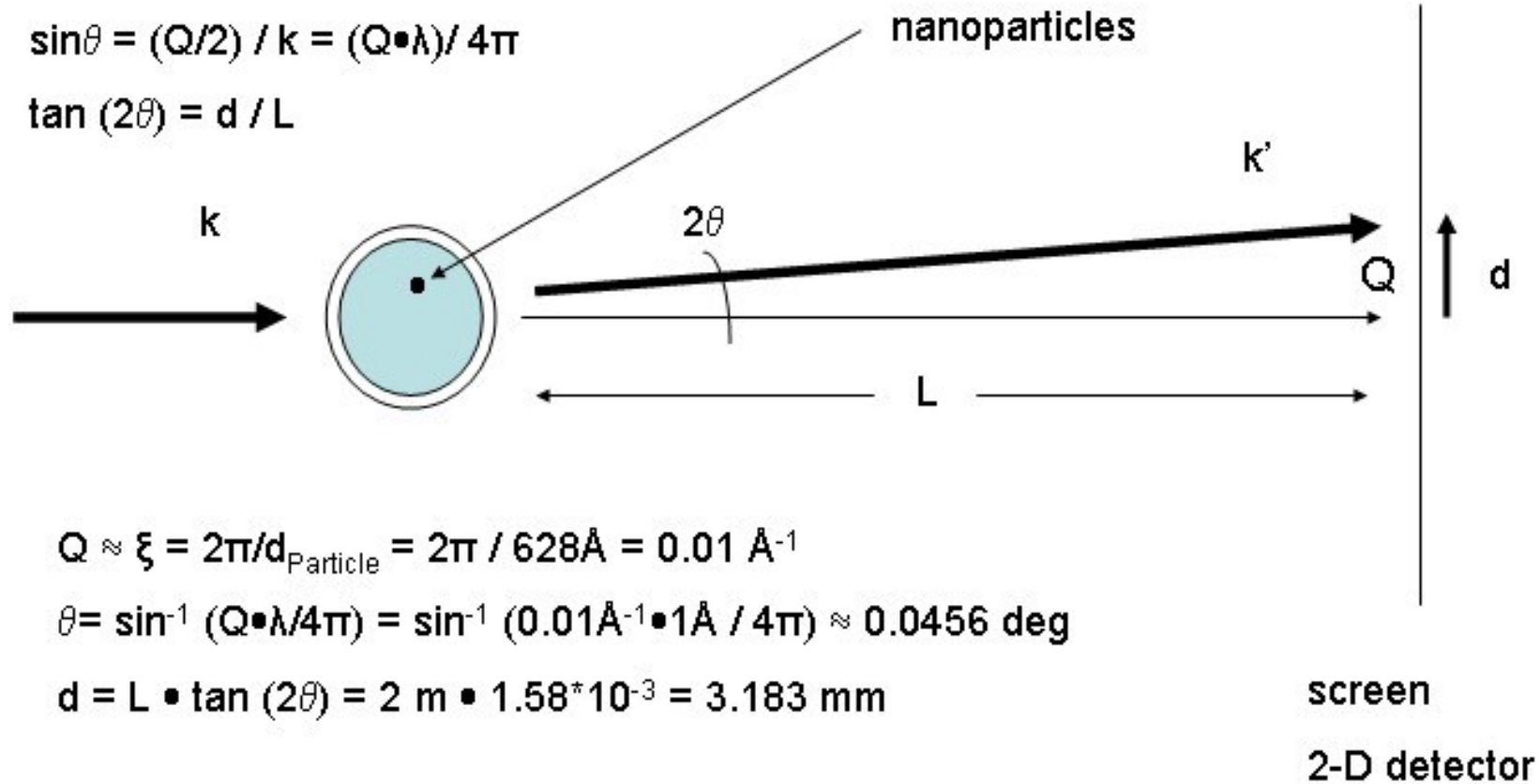
with $J_1(x)$: Bessel function of the first kind.

For $Q \rightarrow 0$: $|F(Q)|^2 = 1$ and $I_{\text{SAXS}}(Q) = \Delta\rho^2 V_p^2$



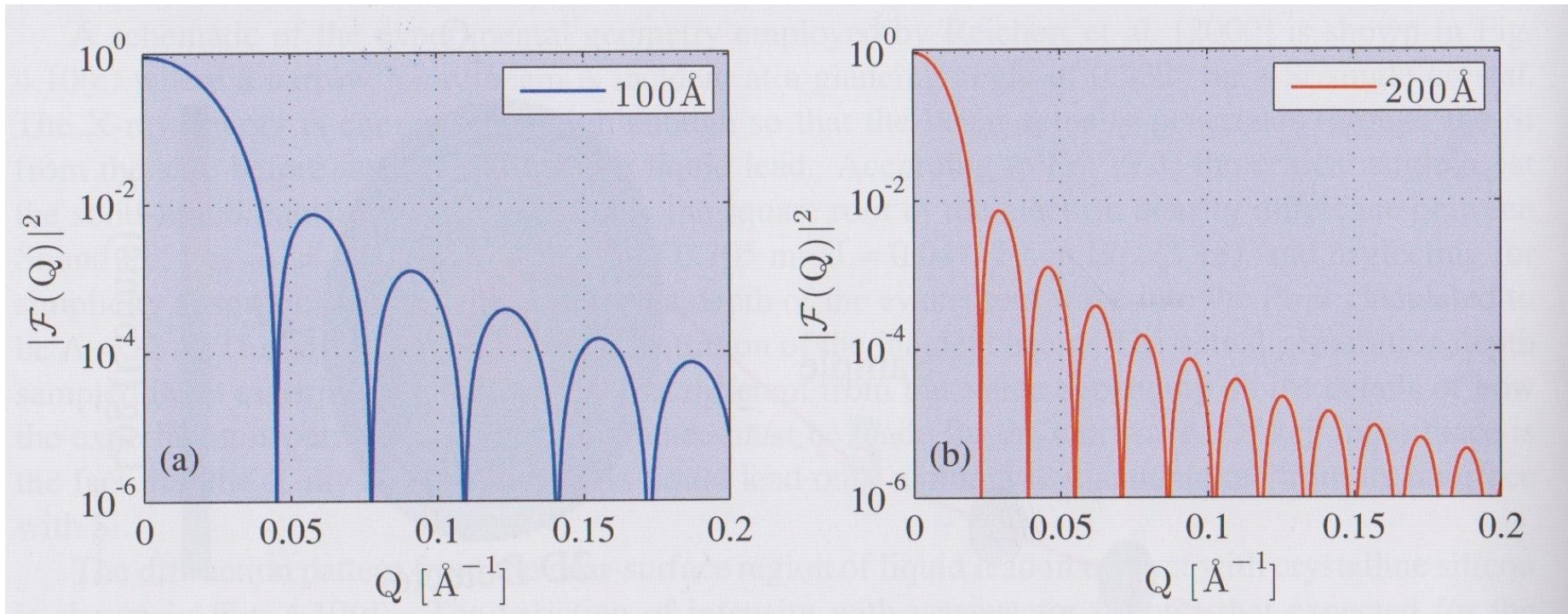
Experimental Set-up (SAXS)

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

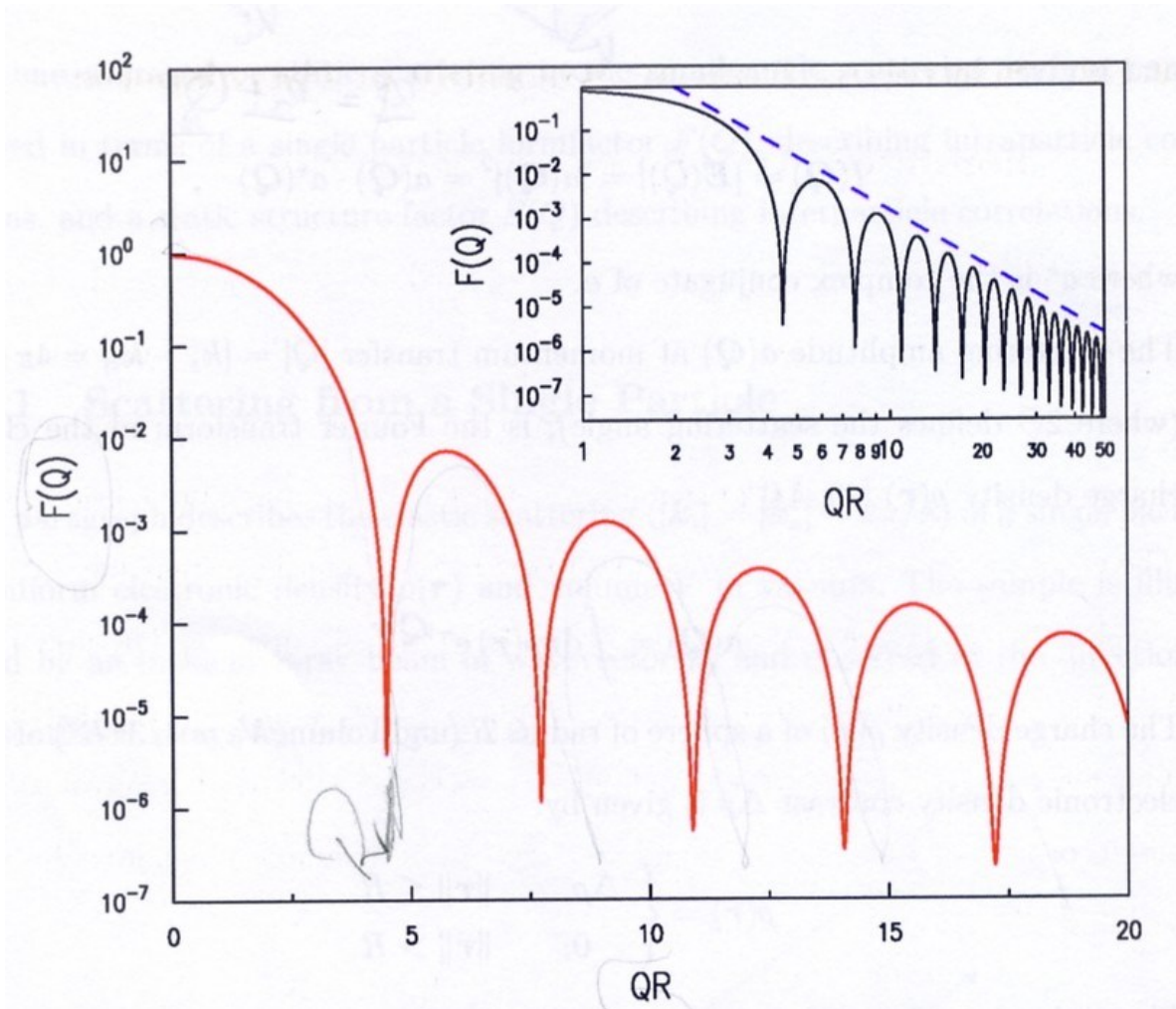


Form Factor for Monodisperse Spheres

Monodisperse spheres of radius 10nm and 20 nm



Form Factor for Monodisperse Spheres



The Small Q Limit: Guinier Regime

For $QR \rightarrow 0$:

$$\begin{aligned}
 F(Q) &\approx \frac{3}{(QR)^3} \left[QR - \frac{(QR)^3}{6} + \frac{(QR)^5}{120} = \dots - QR \left(1 - \frac{(QR)^2}{2} + \frac{(QR)^4}{24} \right) \right] \\
 &\approx 1 - \frac{(QR)^2}{10}
 \end{aligned}$$

Thus:

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

Thus the $QR \rightarrow 0$ limit can be used to determine the particle radius R via:

$$I_{\text{SAXS}}(Q) \approx \Delta\rho^2 V_p^2 e^{-\frac{(QR)^2}{5}} \quad QR \ll 1 \quad [e^{-x} = 1 - x]$$

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



The Large Q Limit: Porod Regime

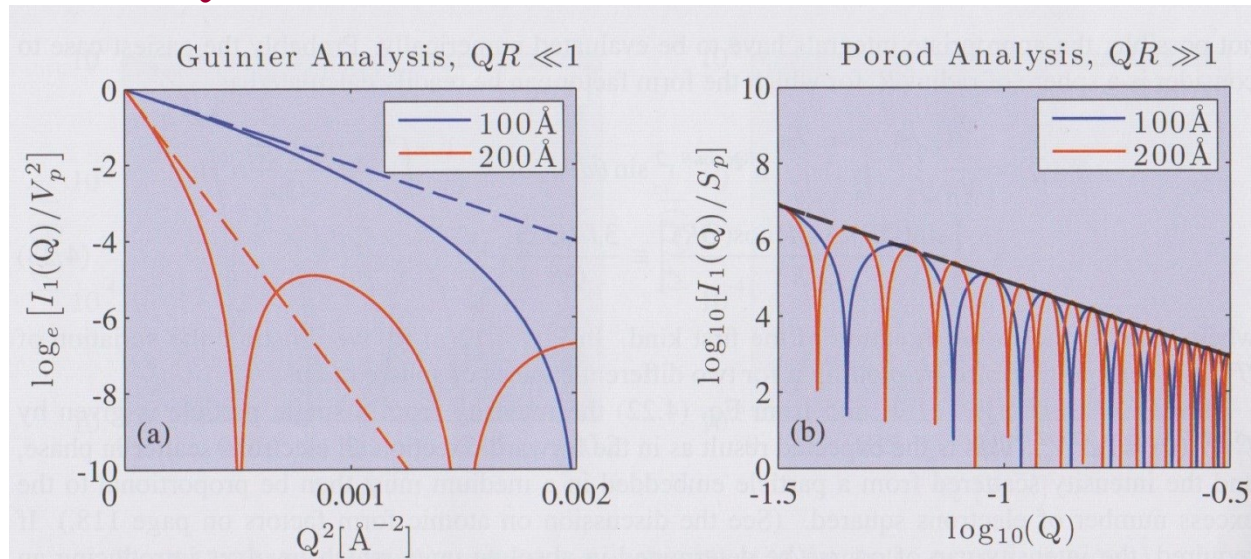
For $QR \gg 1$: wavelength small compared to particle size

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

When $QR \gg 1$ $\cos^2(x)$ oscillates towards $\frac{1}{2}$ and

$$I_{\text{SAXS}}(Q) = 9\Delta\rho^2 V_p^2 \frac{\langle \cos^2(QR) \rangle}{(QR)^4} = \frac{9\Delta\rho^2 V_p^2}{2(QR)^4}$$

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



Radius of Gyration

Radius of gyration: root mean square distance from the particle's center

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

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

For uniform spheres: $R_G^2 = \frac{3}{5} R^2$

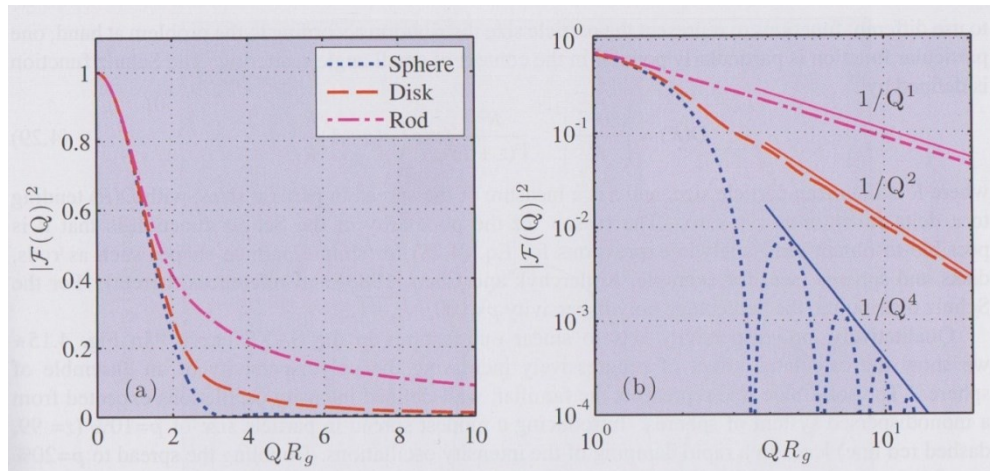
$$I^{SAXS}(Q) \approx \Delta\rho^2 V_P^2 e^{(-QR_G)^2/3}$$

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)	$\frac{2\text{Si}(QL)}{QL} - \frac{4 \sin^2(QL/2)}{(QL)^2}$	$\sqrt{\frac{1}{12}} L$	-1

with: $\text{Si}(x) = \int_0^x \frac{\sin t}{t} dt$



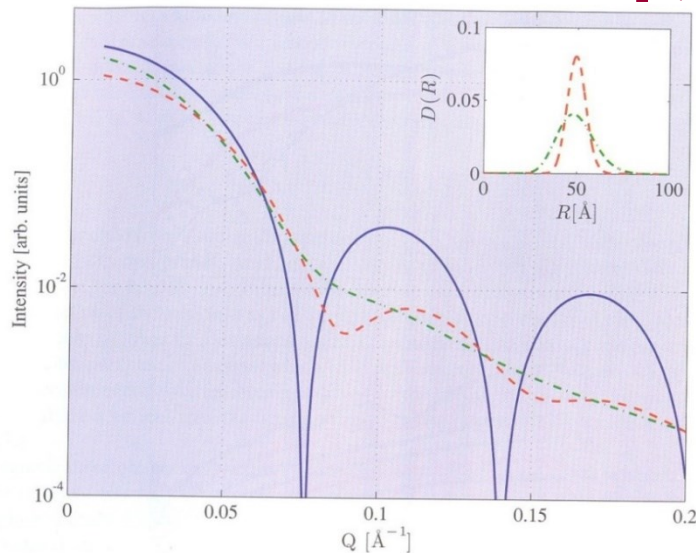
Polydispersity

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

$$I_{\text{SAXS}}(Q) = \Delta\rho^2 \int_0^\infty D(R) V_p^2 |F(Q, R)|^2 dR$$

with $\int_0^\infty D(R) dR = 1$. A frequently used distribution function is the so-called Schultz function, where z is a measure of the polydispersity:

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



Structure Factor

Interparticle interactions:

$S(Q)$: structure factor

Hard sphere structure factor:

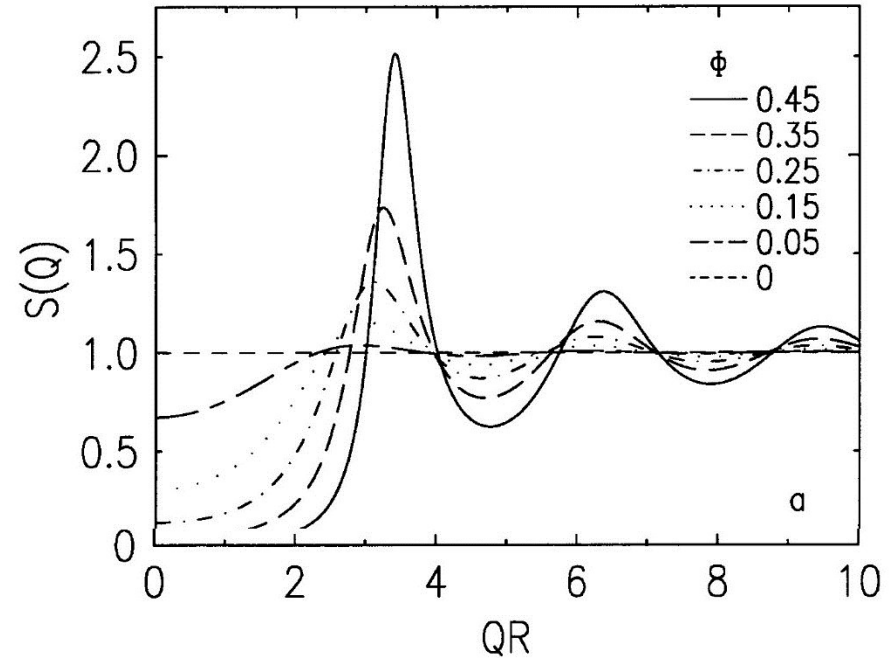
$$V(r) = 0 \quad \text{for } r \geq d$$

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

$$I_{\text{SAXS}}(Q) = \Delta\rho^2 V_p^2 |F(Q)|^2 S(Q)$$

$$S(Q) = \frac{1}{nN} \left\langle \sum_{i,j}^N e^{iQ(R_i - R_j)} \right\rangle$$

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



SAXS Experiment

- measure $I(Q)$
- model $F(Q)$
- for spherical particles $I(Q)=F(Q)\bullet S(Q)$
- get and model $S(Q)$

