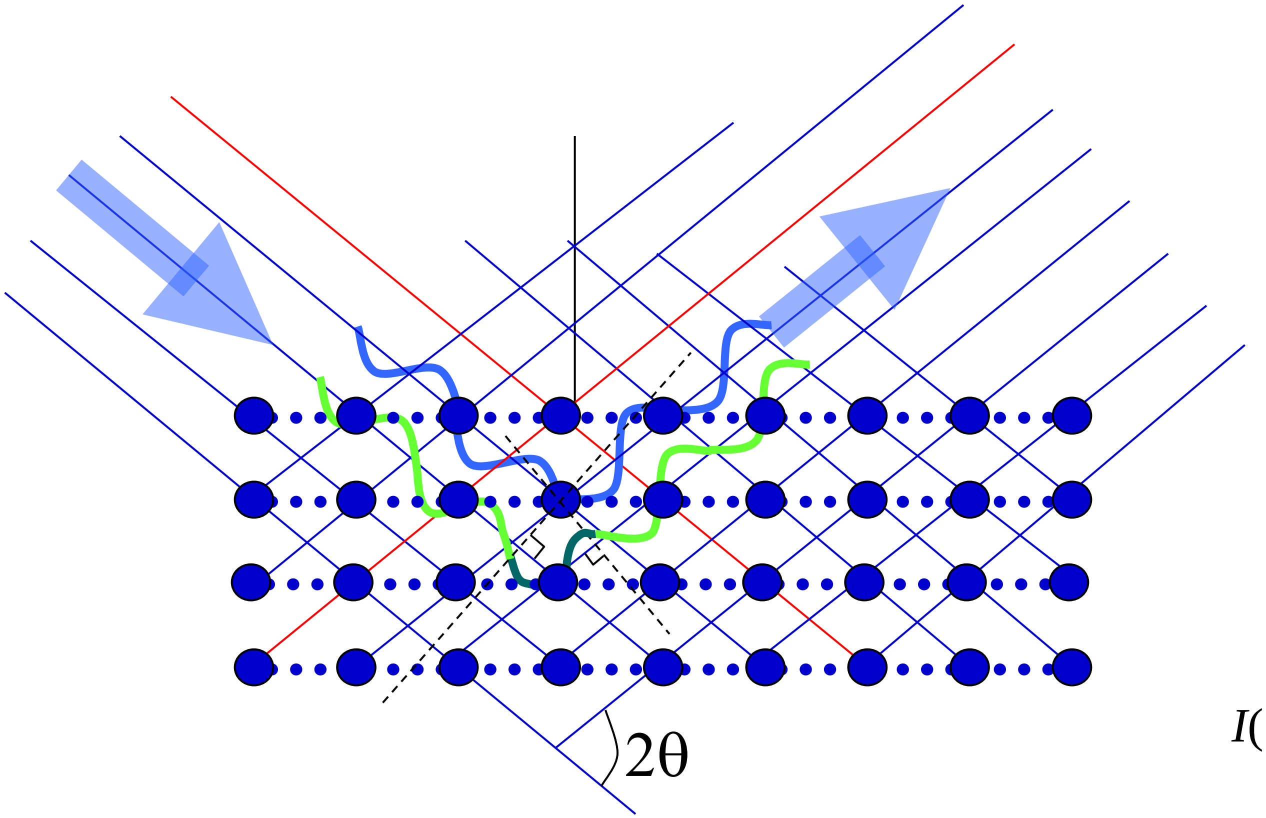
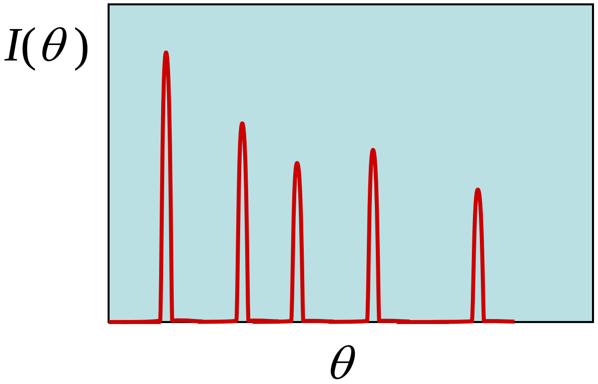
Small-Angle Scattering
Basic Theory

Bragg Scattering

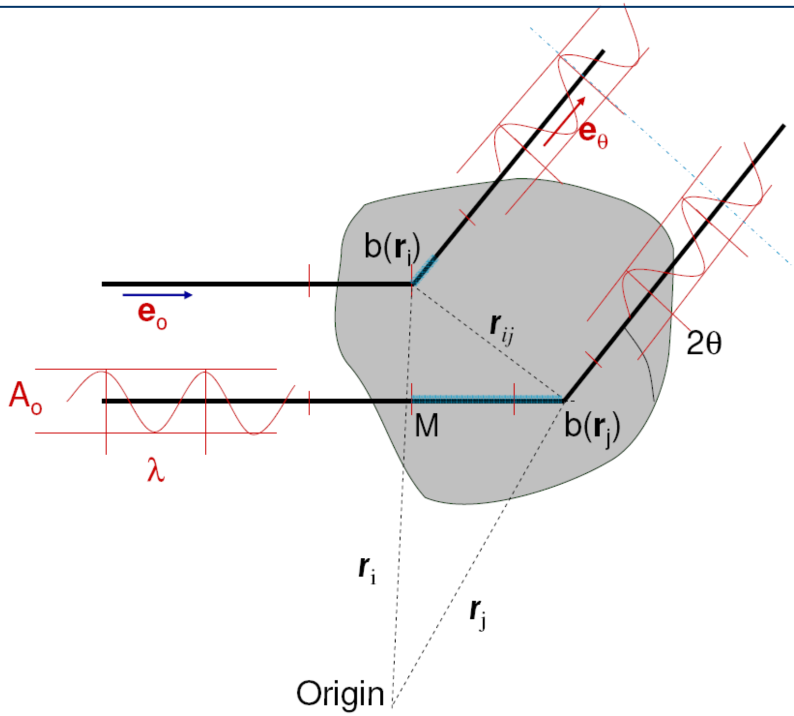
From the periodic lattice of a solid



$$n\lambda = 2d \sin \theta$$



Phase



$$\Delta\phi = |\mathbf{PN} - \mathbf{OM}| \cdot \frac{2\pi}{\lambda}$$

$$\Delta\phi = (\mathbf{r_{ij}} \cdot \mathbf{e}_\theta - \mathbf{r_{ij}} \cdot \mathbf{e_o})\frac{2\pi}{\lambda}$$

$$\mathbf{k_o} = \frac{2\pi}{\lambda}\mathbf{e}_\circ$$

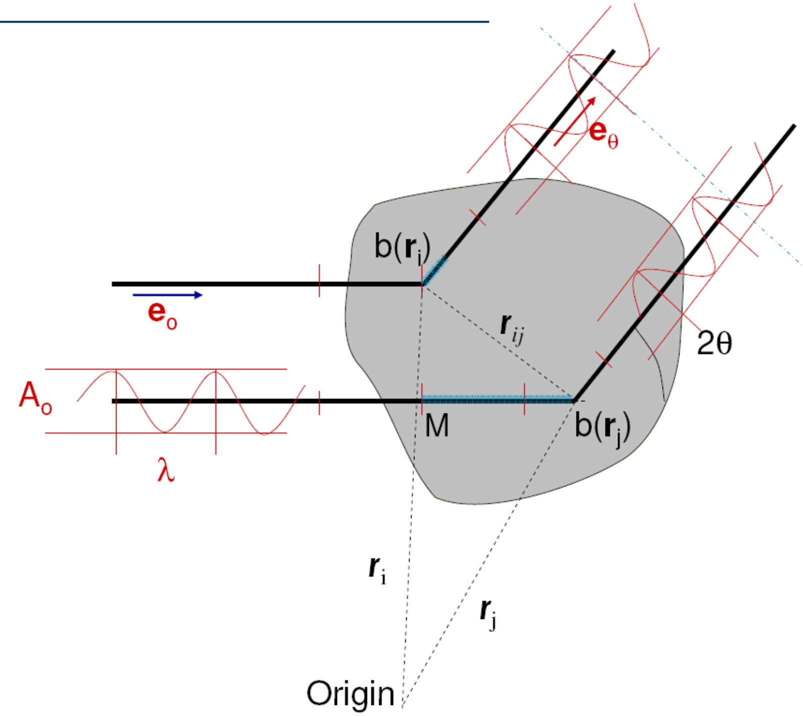
$$\mathbf{k}_\theta = \frac{2\pi}{\lambda}\mathbf{e}_\theta$$

$$\Delta\phi = \mathbf{r}_{ij} \cdot (\mathbf{k}_\theta - \mathbf{k}_\circ) = \mathbf{r}_{ij} \cdot \mathbf{q}$$

$\mathbf{q} = \mathbf{k}_\theta - \mathbf{k}_\circ$ is the *scattering vector*, or *momentum transfer*

$$q = |\mathbf{q}| = \frac{2\pi}{\lambda}|\mathbf{e}_\theta - \mathbf{e}_\circ| = \frac{4\pi}{\lambda}\sin(\theta)$$

Amplitude



Phase difference

$$\Delta\phi = \mathbf{r}_{ij} \cdot (\mathbf{k}_\theta - \mathbf{k}_\circ) = \mathbf{r}_{ij} \cdot \mathbf{q}$$

Amplitude

$$A(t, \boldsymbol{r}) = A_o \exp[i(\omega t - \boldsymbol{k} \cdot \boldsymbol{r})]$$

Scattering from site $\mathbf{r_i}$ into angle 2θ, or better scattering vector $\mathbf{q}$

$$\begin{aligned} A(\mathbf{q})_{\mathbf{r}_i} &= A_\circ \mathrm{b}(\mathbf{r}_i) \exp[i(\omega t - \Delta\phi - \mathbf{k}_\theta \cdot \mathbf{r})] \\ &= A_\circ \mathrm{b}(\mathbf{r}_i) \exp[i(\omega t - \mathbf{q} \cdot \mathbf{r}_i - \mathbf{k}_\theta \cdot \mathbf{r})] \\ &= A_\circ \mathrm{b}(\mathbf{r}_i) \exp[-i(\mathbf{q} \cdot \mathbf{r}_i)] \ \exp[i(\omega t - \mathbf{k}_\theta \cdot \mathbf{r})] \end{aligned}$$

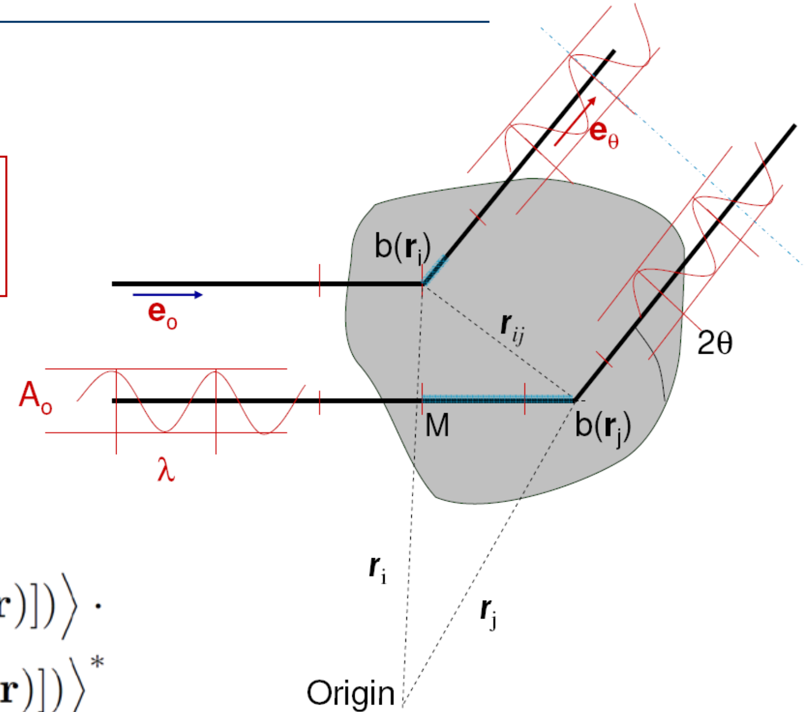
Sample

$$\boxed{A(\mathbf{q}) = A_\circ \sum_{sample} \mathrm{b}(\mathbf{r}_i) \exp[-i(\mathbf{q} \cdot \mathbf{r}_i)] \ \exp[i(\omega t - \mathbf{k}_\theta \cdot \mathbf{r})]}$$

Amplitude -> Intensity

Scattering-Amplitude from sample A(**q**)

$$A(\mathbf{q}) = A_\circ \sum_{sample} \mathrm{b}(\mathbf{r}_i) \exp[-i(\mathbf{q}\cdot\mathbf{r}_i)] \;\; \exp[i(\omega t - \mathbf{k}_\theta \cdot \mathbf{r})]$$



Intensity

$$\begin{aligned}
\tilde{I}(\mathbf{q}) &= A_\circ \Big\langle \big(\sum \mathrm{b}(\mathbf{r}_i) \exp[-i(\mathbf{q}\cdot\mathbf{r}_i)] \exp[i(\omega t - \mathbf{k}_\theta \cdot \mathbf{r})]\big) \Big\rangle \cdot \\
& \quad A_\circ \Big\langle \big(\sum \mathrm{b}(\mathbf{r}_j) \exp[-i(\mathbf{q}\cdot\mathbf{r}_j)] \exp[i(\omega t - \mathbf{k}_\theta \cdot \mathbf{r})]\big) \Big\rangle^* \\
&= A_\circ^2 \langle \sum_i \sum_j \mathrm{b}(\mathbf{r}_i)\mathrm{b}(\mathbf{r}_j) \exp[-i(\mathbf{q}\cdot\mathbf{r}_{ij})] \rangle \\
&= I_\circ \sum_i \sum_j \langle \mathrm{b}(\mathbf{r}_i)\mathrm{b}(\mathbf{r}_j) \;\; \exp[-i(\mathbf{q}\cdot\mathbf{r}_{ij})] \rangle
\end{aligned}$$

average

Measured Intensity $\tilde{I}(\boldsymbol{q})$

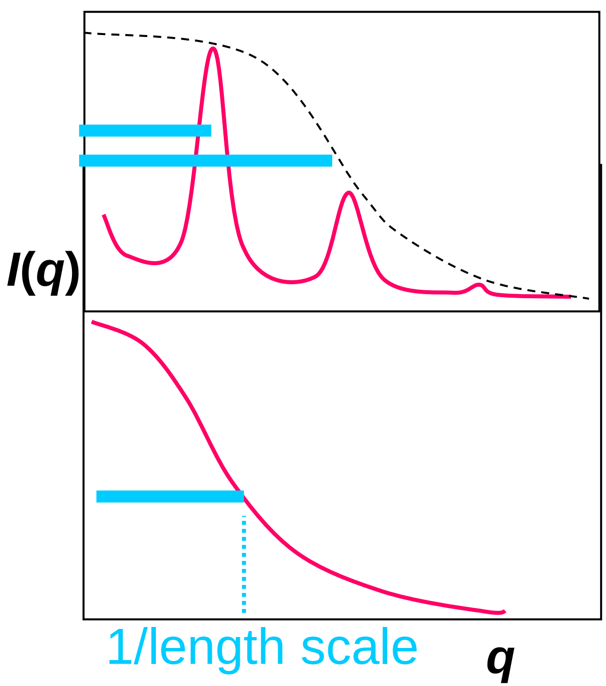
Scattering Function $I(\boldsymbol{q}) = \dfrac{d\sigma}{d\Omega} = \tilde{I}(\boldsymbol{q})/I_o$

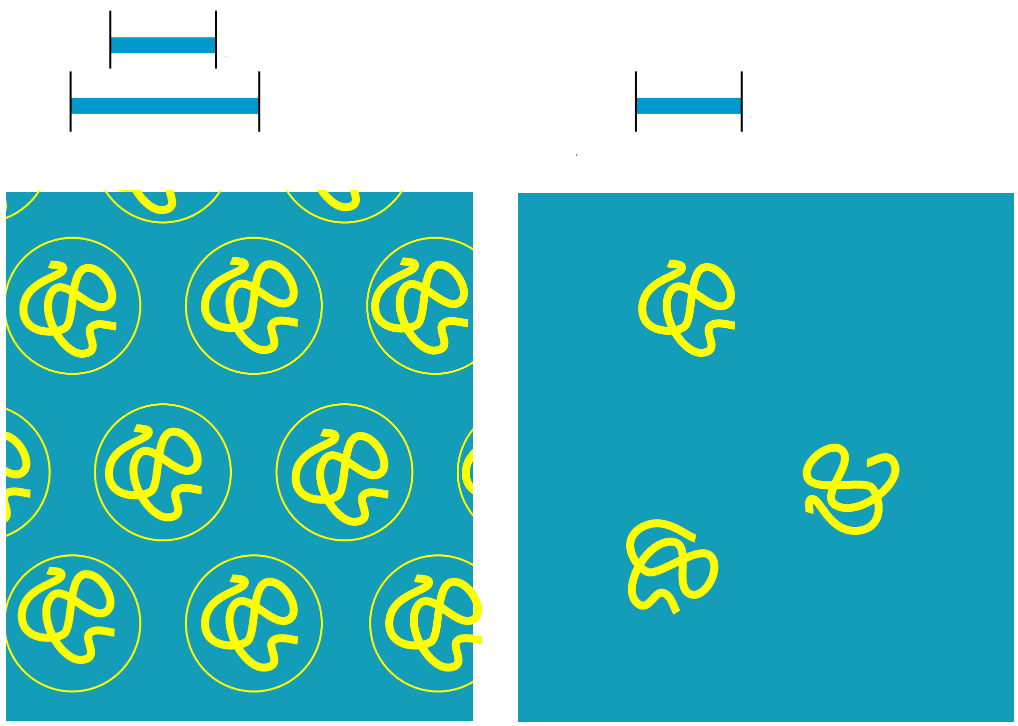
Small-Angle Scattering; Length scale

- Neutron: SANS 10-1000Å
- X-ray: SAXS 10-1000Å
- Light: SALS 0.1-100mm
  - type depending on
    - length scale
    - contrast
    - sample environment

Scattered intensity given by correlations

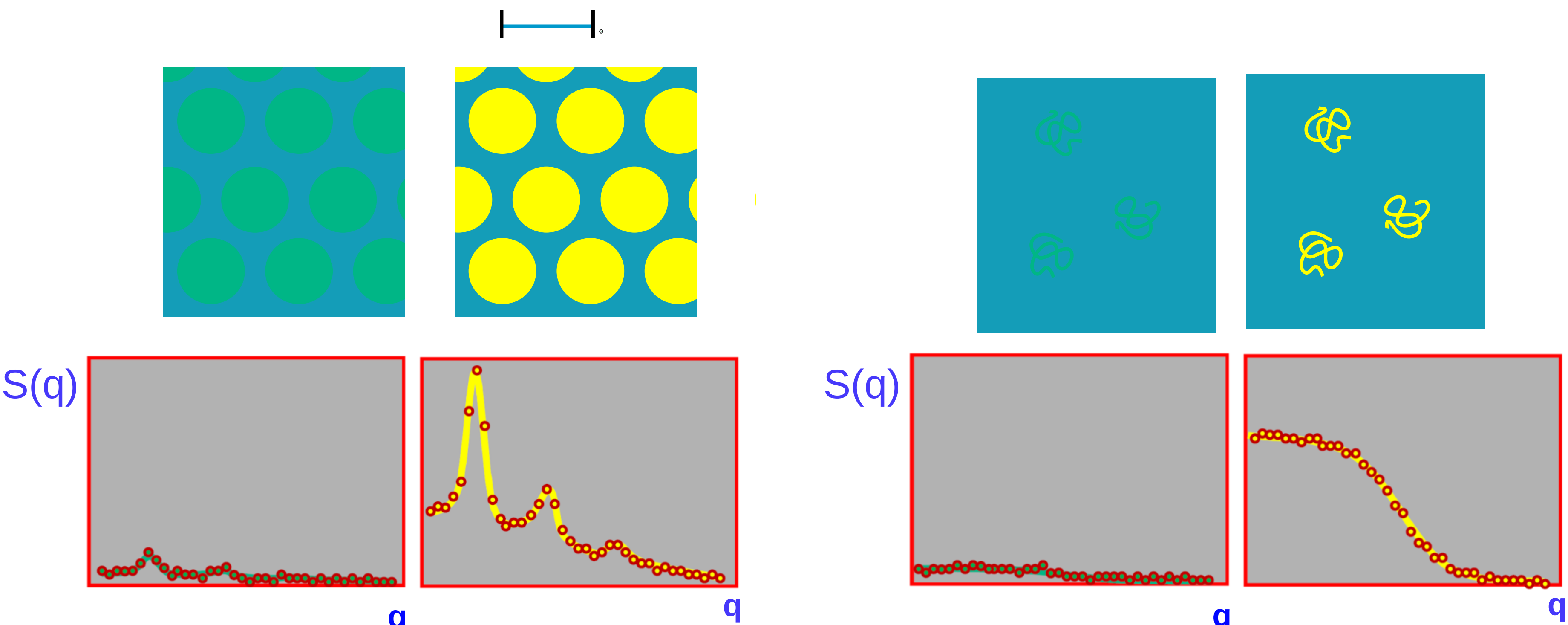
$$I(q) = \int\int \rho_i \rho_j \exp\left(i\overline{q}\cdot\overline{r_{ij}}\right) d^3r_i d^3r_j$$





Small-Angle Scattering, CONTRAST

- Neutron: SANS 10-1000Å
- X-ray: SAXS 10-1000Å
- Light: SALS 0.1-100μm
  - type depending on
    - length scale
    - contrast
    - sample environment



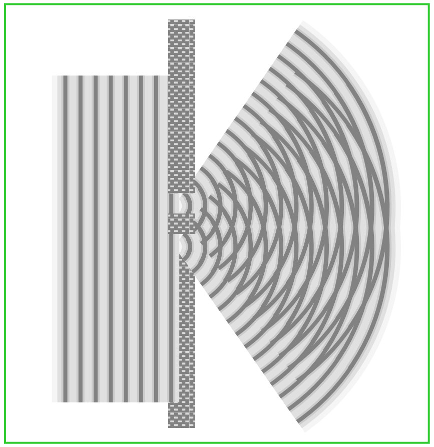
Scattering cross-section

neutrons

NEUTRONS

The interaction between matter and neutrons

The neutron treated as a planar wave with wavelength λ through the de Broglie relation



$$\lambda = \frac{h}{m_n \; v_n}$$

where the velocity v_n is given by the thermal energy $E_n = k_B T$ as

$$v_n = \sqrt{k_B T / m_n}$$

for thermal energies	$T \sim 300$K,
the neutron velocity is of the order of	3000 m/s
and the neutron wavelength of the order of	1.4Å

The neutron scattering length

www.ncnr.nist.gov/resources/n-lengths

Nuclei	Coherent Scattering Length b_i	Incoherent Cross Section $sigma_{ic}$
H	$-0.3739 \cdot 10^{-12}$cm	$80.26 \cdot 10^{-24}$cm^2
^{1}H	$-0.3741 \cdot 10^{-12}$cm	$80.27 \cdot 10^{-24}$cm^2
^{2}H $=$ D	$0.6671 \cdot 10^{-12}$cm	$2.05 \cdot 10^{-24}$cm^2
C	$0.6646 \cdot 10^{-12}$cm	$0.001 \cdot 10^{-24}$cm^2
^{12}C	$0.6651 \cdot 10^{-12}$cm	$0 \cdot 10^{-24}$cm^2
N	$0.936 \cdot 10^{-12}$cm	$0.50 \cdot 10^{-24}$cm^2
^{14}N	$0.937 \cdot 10^{-12}$cm	$0.50 \cdot 10^{-24}$cm^2
O	$0.5803 \cdot 10^{-12}$cm	$0.0 \cdot 10^{-24}$cm^2
^{16}O	$0.5803 \cdot 10^{-12}$cm	$0.0 \cdot 10^{-24}$cm^2
Si	$0.4149 \cdot 10^{-12}$cm	$0.004 \cdot 10^{-24}$cm^2
^{28}Si	$0.4107 \cdot 10^{-12}$cm	$0 \cdot 10^{-24}$cm^2
Cl	$0.958 \cdot 10^{-12}$cm	$5.3 \cdot 10^{-24}$cm^2
^{35}Cl	$1.165 \cdot 10^{-12}$cm	$4.7 \cdot 10^{-24}$cm^2
Ca	$0.479 \cdot 10^{-12}$cm	$0.05 \cdot 10^{-24}$cm^2
^{40}Ca	$0.480 \cdot 10^{-12}$cm	$0 \cdot 10^{-24}$cm^2

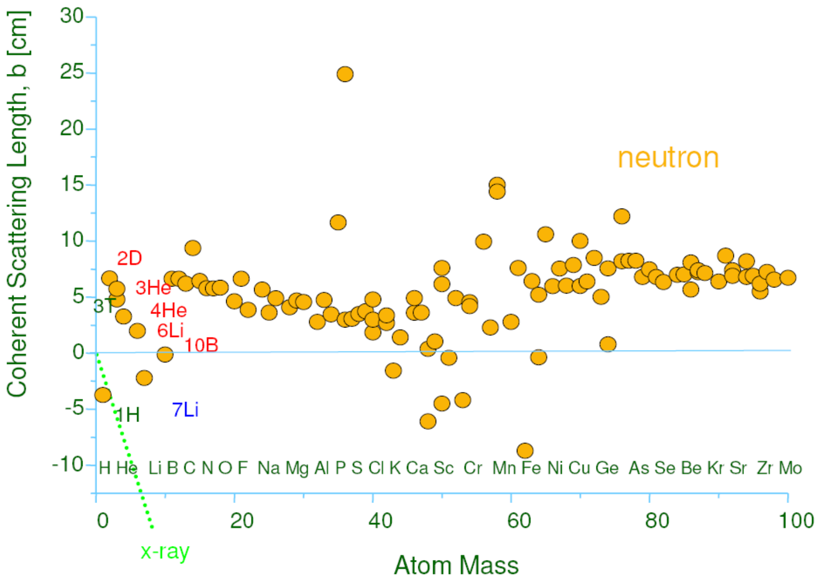
The interaction between matter and neutrons

1. Interaction with Nuclei

Two different interaction terms, if the nucleus spin is finite

The average coupling gives coherent scattering

The deviation from average gives incoherent scattering



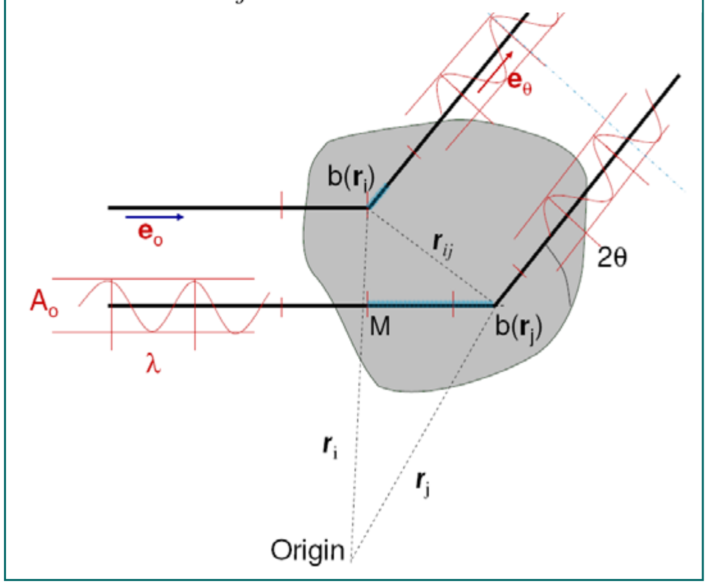
Nuclei	**Coherent Scattering Length**	**Incoherent Cross Section**
^{1}H	$-0.374 \cdot 10^{-12}$ cm	$79.9 \cdot 10^{-24}$ cm^2
^{2}D	$0.667 \cdot 10^{-12}$ cm	$2.04 \cdot 10^{-24}$ cm^2
^{16}O	$0.580 \cdot 10^{-12}$ cm	$0.0009 \cdot 10^{-24}$ cm^2
^{12}C	$0.665 \cdot 10^{-12}$ cm	$0.001 \cdot 10^{-24}$ cm^2

2. Interaction with Magnetic Moment (electrons)

……

The neutron scattering length density

$$I(\mathbf{q}) = \sum_i \sum_j \langle \mathrm{b}(\mathbf{r}_i)\mathrm{b}(\mathbf{r}_j) \exp[-i(\mathbf{q}\cdot\mathbf{r})] \rangle$$



q small, i.e. r large for a given value of qr
With maximum: q_{max} ~ 0.5Å^{-1},
we have a lower-size resolution of the order of

$r \sim 2\pi / q_{\mathrm{max}} \sim 10$Å.

i.e. molecular, but not atomic scale resolution.

$$\mathrm{b}_i \rightarrow \rho(\mathbf{r}_i) d\mathbf{r}_i$$

Define continuum parameter:
scattering length density

$$\boxed{\rho = \frac{1}{V} \sum_V \mathrm{b}_i = \frac{N_A \delta}{M_V} \sum_V \mathrm{b}_i}$$

Substitute scattering length with scattering length density:

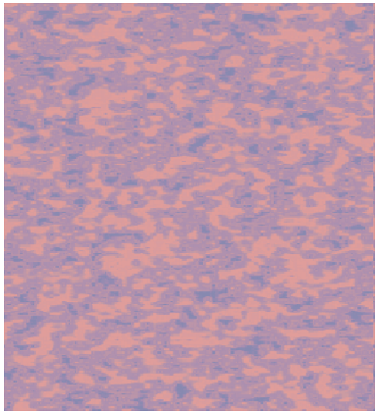
$$\begin{aligned} I(\mathbf{q}) &= \int_{\mathbf{R}_i} \int_{\mathbf{R}j} \langle \rho(\mathbf{R}_\mathrm{i}) \rho(\mathbf{R}_\mathrm{j}) \rangle \exp[-i\mathbf{q}\cdot\mathbf{r}_{\mathrm{ij}}]\, d\mathbf{R}_\mathrm{j}\, d\mathbf{R}_\mathrm{i} \\ &= \int_{\mathbf{R}} \int_{\mathbf{r}} \langle \rho(\mathbf{R}) \rho(\mathbf{R}+\mathbf{r}) \rangle \exp[-i\mathbf{q}\cdot\mathbf{r}]\, d\mathbf{r}\, d\mathbf{R} \end{aligned}$$

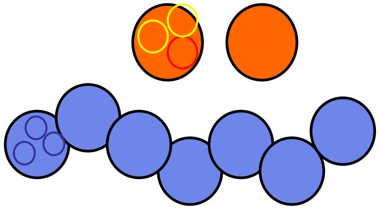
$$\begin{aligned} I(\mathbf{q}) &= V \cdot \int \langle \rho(\mathbf{R}) \rho(\mathbf{R}+\mathbf{r}) \rangle \exp[-i\mathbf{q}\cdot\mathbf{r}]\, d\mathbf{r} \\ &= V \cdot \int \gamma(\mathbf{r}) \exp[-i\mathbf{q}\cdot\mathbf{r}]\, d\mathbf{r} \end{aligned}$$

The scattering length density

Wide-angle diffraction high-resolution
(Atomic length scale)

Small-angle diffraction, low-resolution
(Molecular length-scale)





$$\boxed{\rho = \frac{1}{V}\sum_{V} \mathrm{b}_i = \frac{N_A \delta}{M_V}\sum_{V} \mathrm{b}_i}$$

http://sld-calculator.appspot.com/save

http://www.ncnr.nist.gov/resources/sldcalc.html

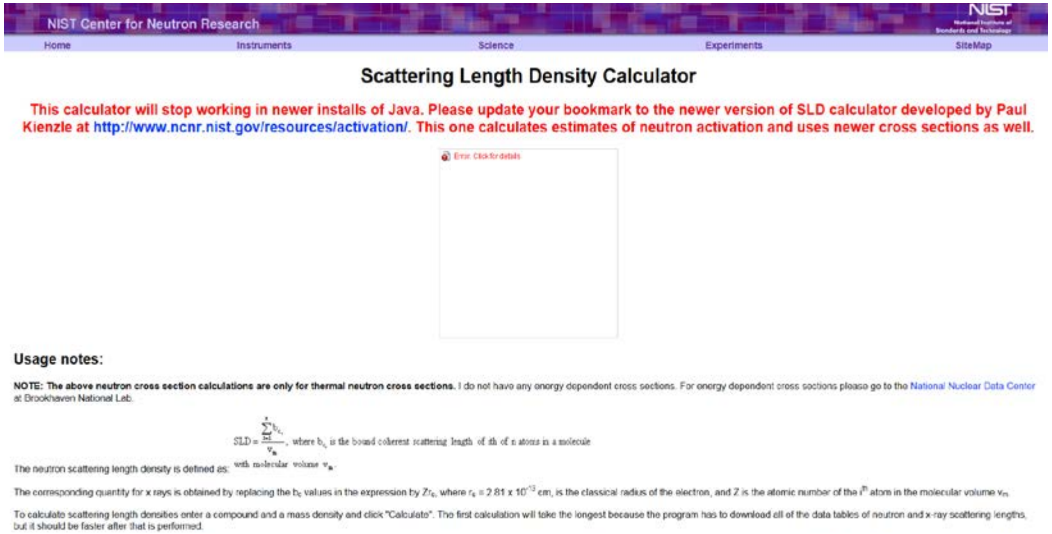
http://www.ncnr.nist.gov/resources/n-lengths/

$$\rho_{\text{water}} = \frac{1}{V_{\text{water}}}(2b_{\mathrm{H}} + b_{\mathrm{O}})$$

$$\rho_{\text{water}} = 6.02 \cdot 10^{23}/\text{mol} \cdot \frac{1\text{g/cm}^3}{18\ \text{g/mol}} \cdot (2 \cdot (-0.374)\ + 0.580) \cdot 10^{-12}\text{cm}$$

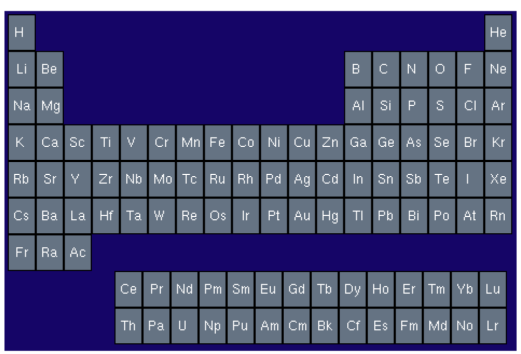
$$\rho_{\text{water}} = -5.62 \cdot 10^9/\text{cm}^2$$

http://www.ncnr.nist.gov/resources/sldcalc.html

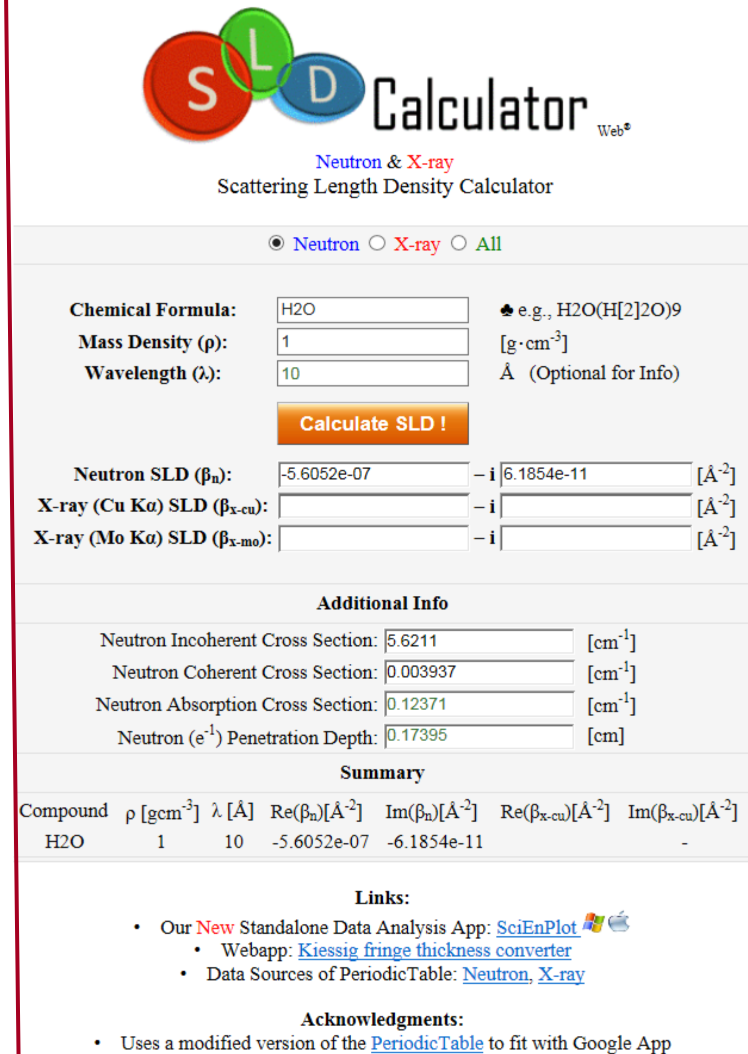


http://www.ncnr.nist.gov/resources/n-lengths/

Neutron scattering lengths and cross sections

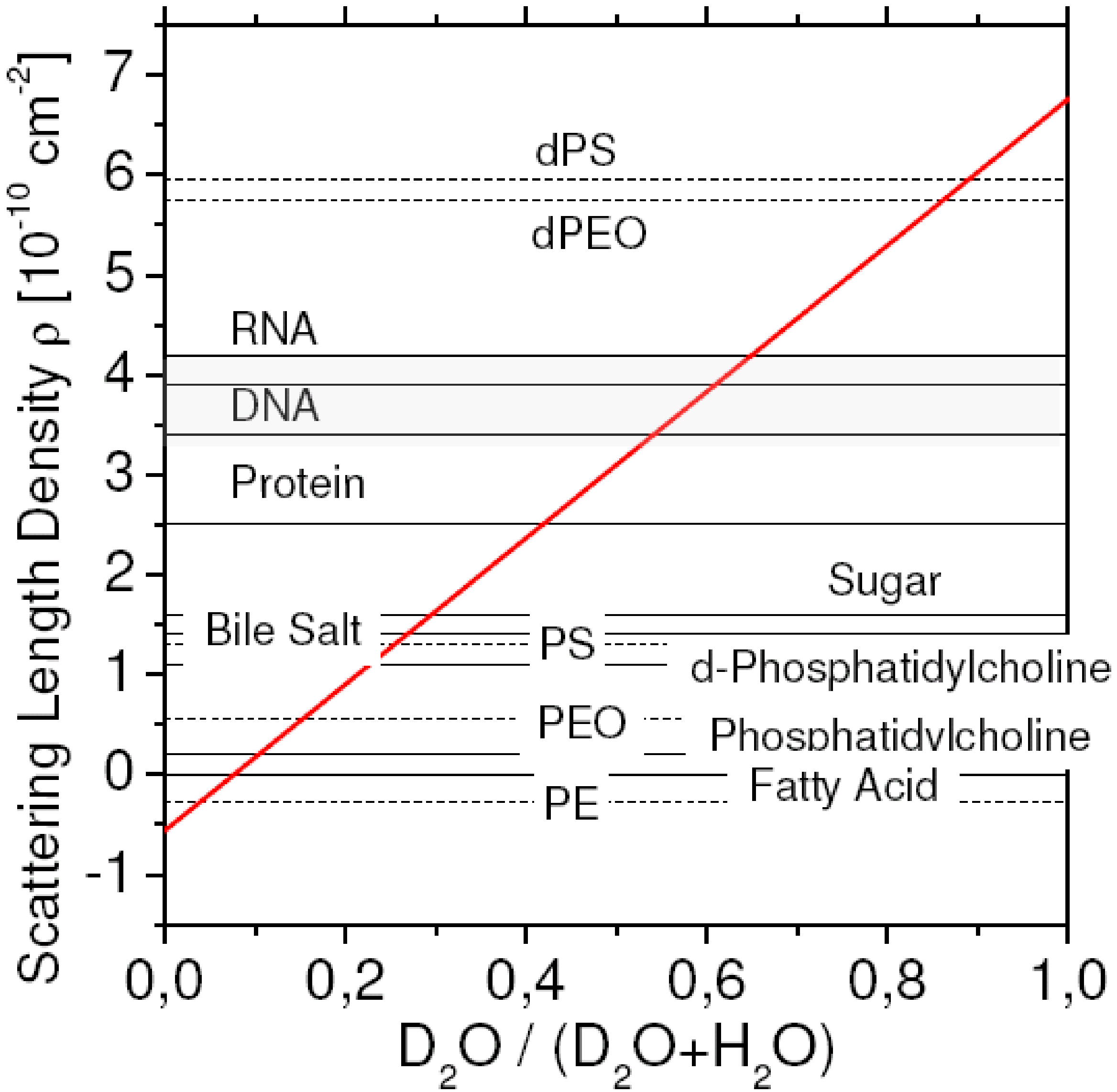


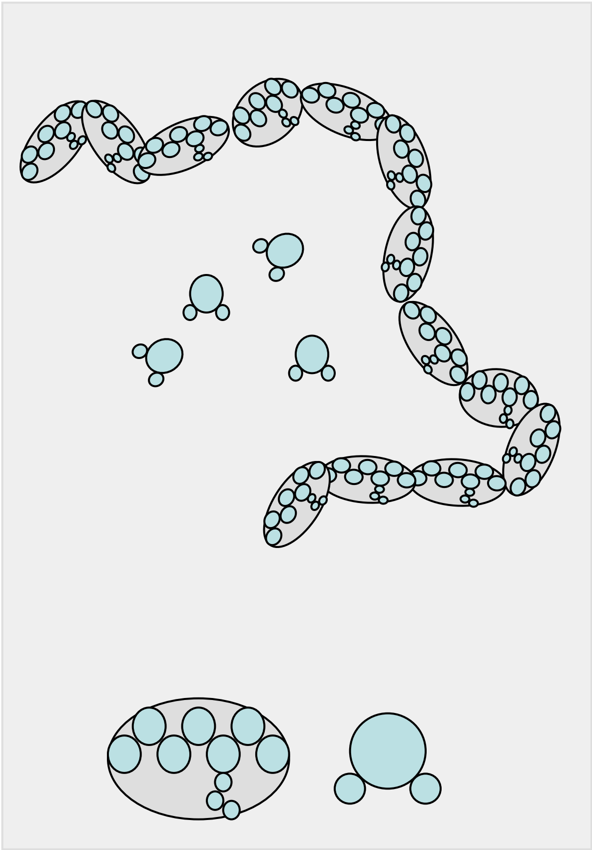
http://sld-calculator.appspot.com/save



Scattering length density

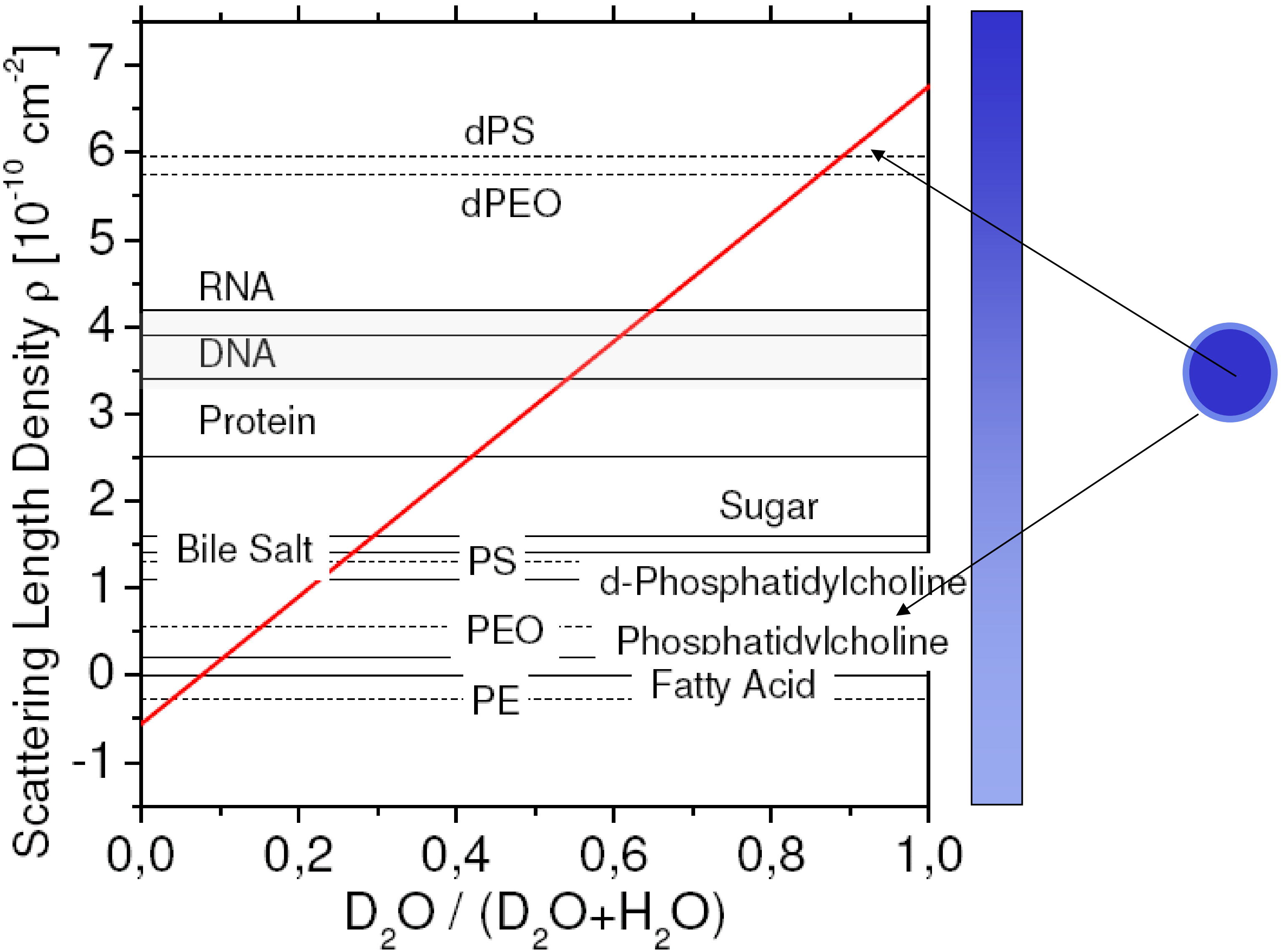
$$\rho = \Sigma b_i / V$$



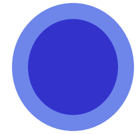


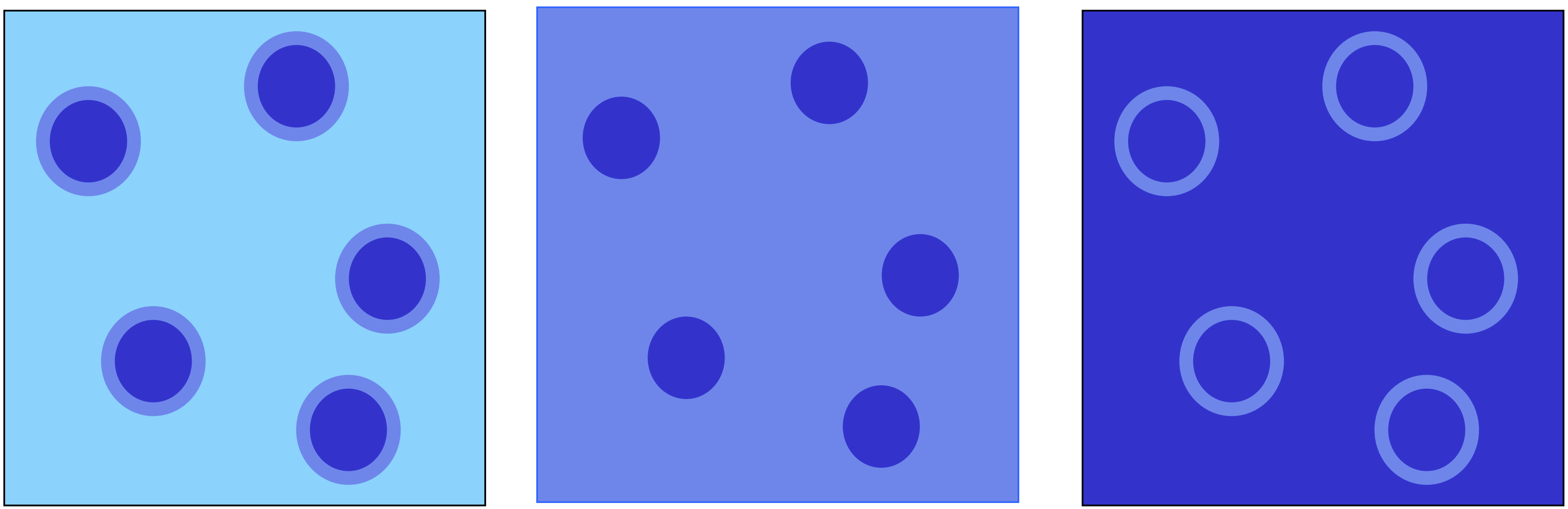
Scattering length density

$\rho = \Sigma b_i / V$



Contrast variation,
- changing solvent

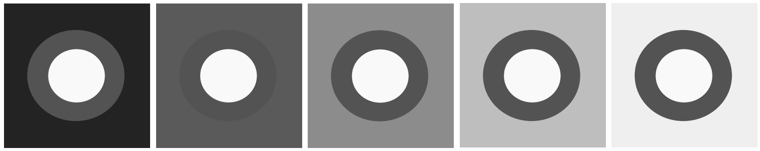




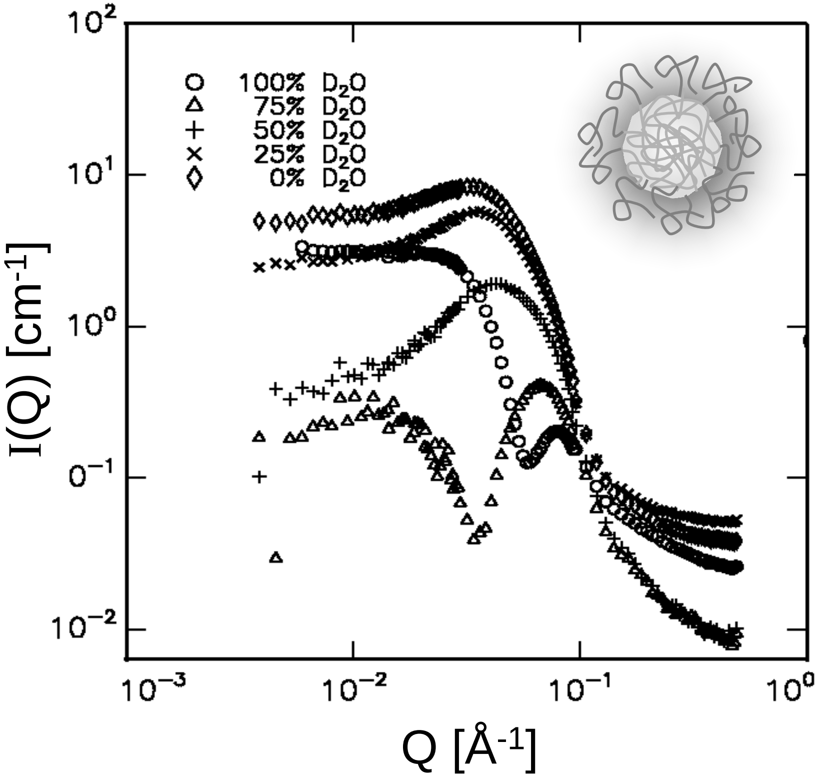
Mixed contrast | Bulk contrast | Interface contrast

Contrast variation changing solvent

Example



Varying D_2O/H_2O ratio



Block copolymer micelles
in water, measured with different D2O/H2O compositions

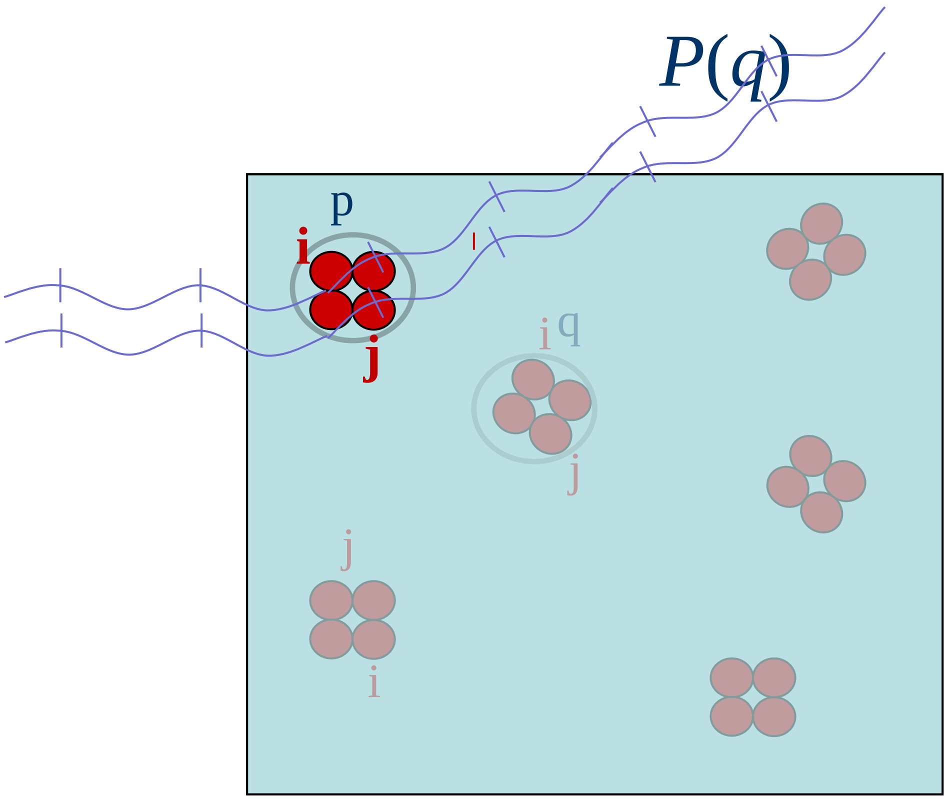
Scattering Function
(Scattering Cross-Section)

Decomposed into

Pre-Factor
Form Factor
Structure Factor

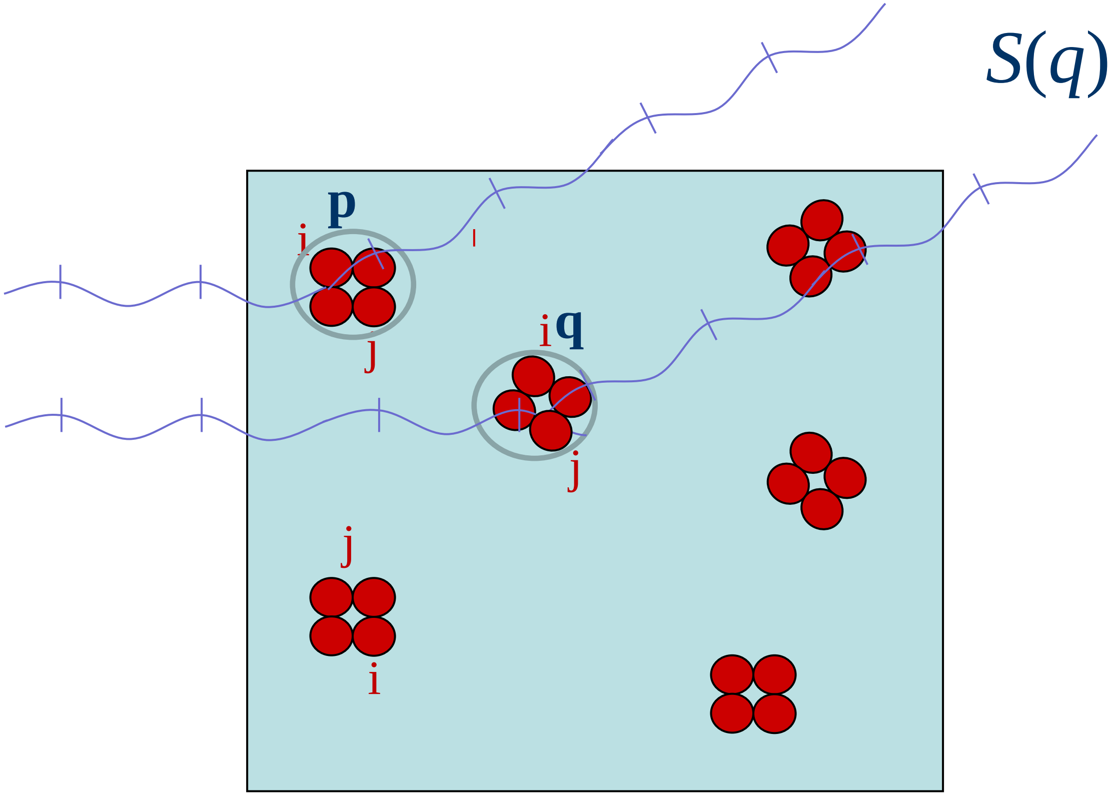
Decomposition into intra and inter correlations

n particles (p,q, ..) with
M subunits (i,j, ..) in each



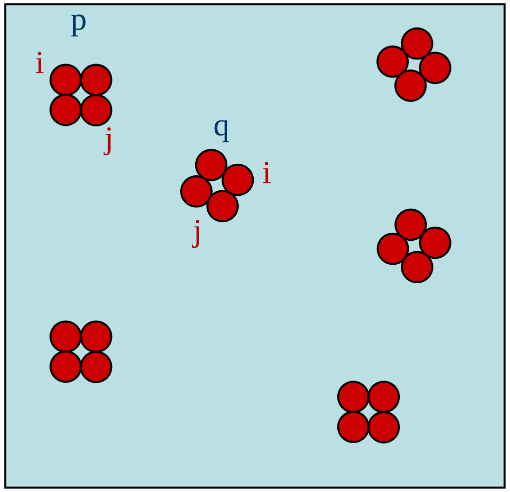
Decomposition into intra and inter correlations

n particles (p,q, ..) with
M subunits (i,j, ..) in each



Decomposition into intra and inter correlations

$$I(\mathbf{q}) = \sum_{i=1}^{M}\sum_{j=1}^{M}\sum_{p=1}^{n}\sum_{q=1}^{n}\left\langle(\Delta\rho)^2 \ \exp[-i\mathbf{q}\cdot(\mathbf{r}_{p,i}-\mathbf{r}_{q,j})]\right\rangle$$



assume spherical symmetry,
dilute mono-disperse ensemble

$$I(\mathbf{q}) \quad = \quad (\Delta\rho)^2 \ nM^2 \cdot \frac{1}{M^2}\sum_{i,j}\left\langle\exp[-i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)]\right\rangle \left[1 + \frac{1}{n}\sum_{p\neq q}\left\langle\exp[-i\mathbf{q}\cdot(\mathbf{r}_p-\mathbf{r}_q)]\right\rangle\right]$$

intra particle correlations giving information on particle shape

inter particle correlations approach 1 for dilute systems

$$I(\mathbf{q}) = \boxed{(\Delta\rho)^2 \ nM^2}\,\boxed{P(\mathbf{q})}\,\boxed{S(\mathbf{q})}$$

pre factor

form factor

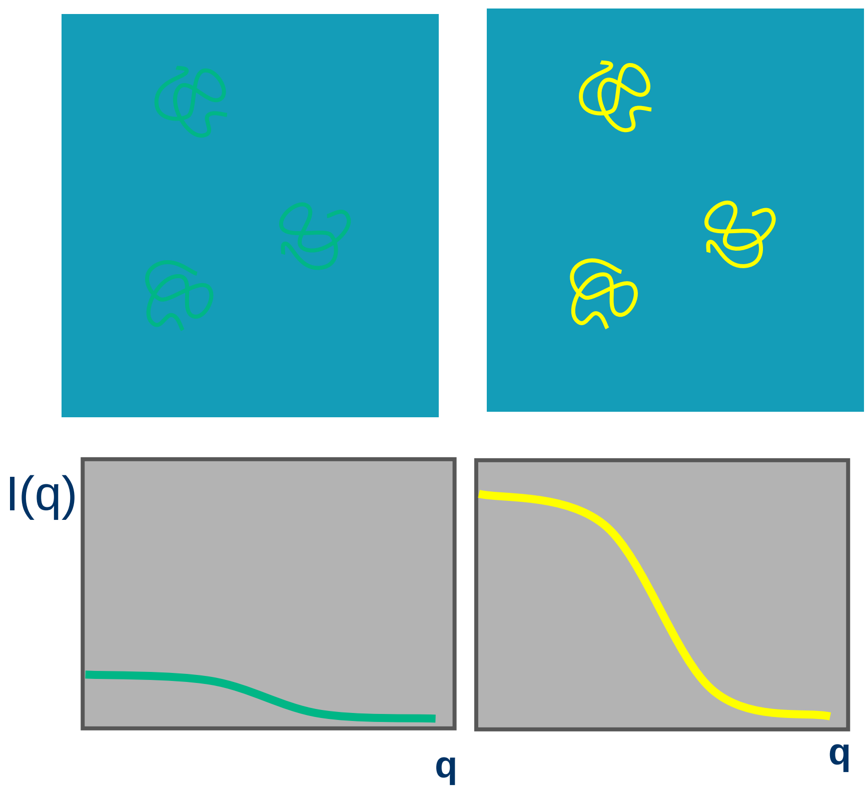
structure factor

P(q) normalized: P(0)=1
S(q)=1 for dilute suspensions

Pre-Factor

Pre-Factor

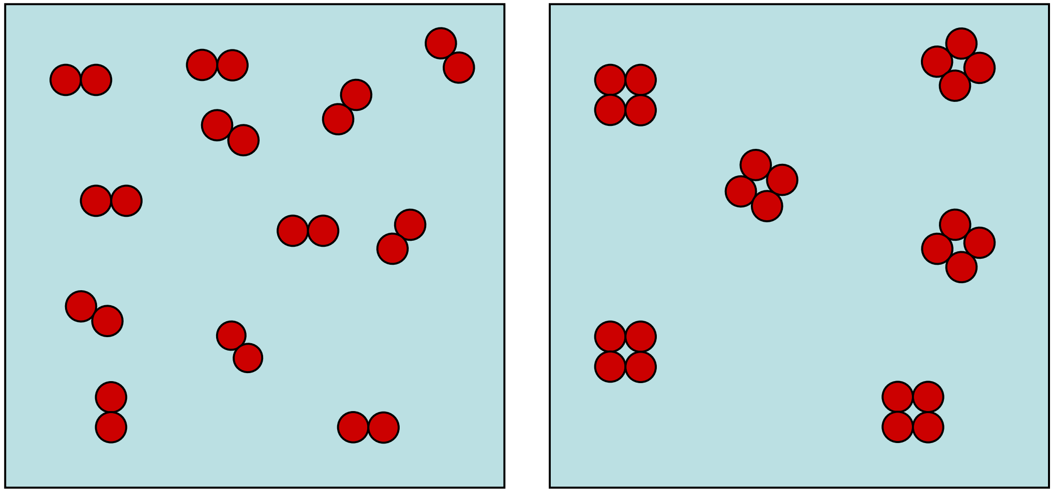
$$I(\mathbf{q}) = \boxed{(\Delta\rho)^2\, nM^2}\, P(\mathbf{q}) S(\mathbf{q})$$



Pre-Factor given by

- Contrast Factor
- Number of Particles
- Mass of Particles

$$I(q) = n\ M^2(\Delta\rho)^2\ P(q)$$



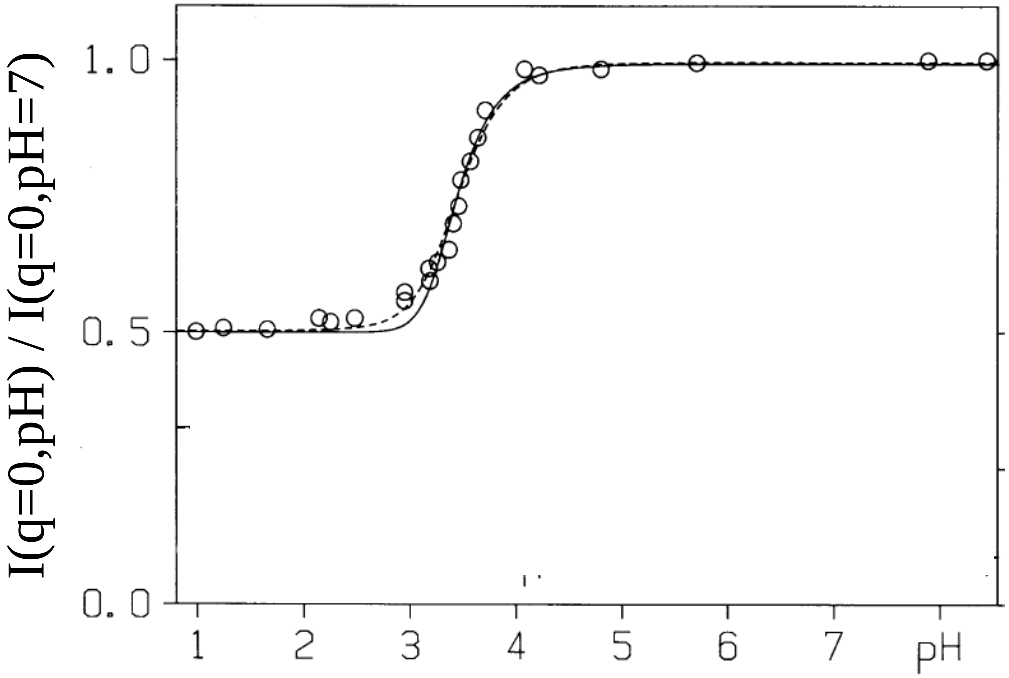
$$pH = 7 \rightarrow pH = 4$$

$$n \rightarrow 2n$$

$$I_{pH=4} \rightarrow$$

$$I_{pH=7} \cdot 2 \cdot \left(\tfrac{1}{2}\right)^2 \cdot 1 \cdot 1$$

$$= \tfrac{1}{2} I_{pH=7}$$

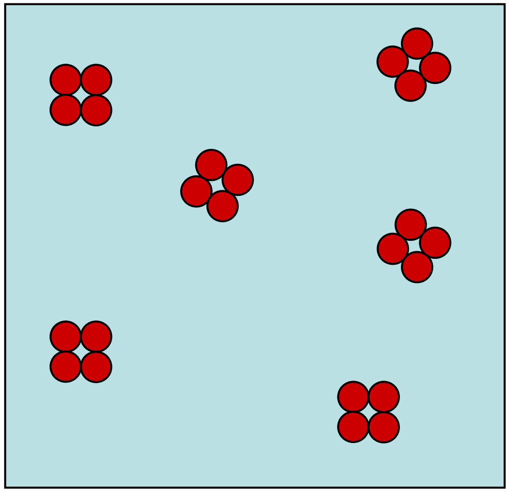


Pap, Sjöberg Mortensen Eur. J Biochem 191 41 (1990)

Form Factor

Decomposition into intra and inter correlations

$$I(\mathbf{q}) = \sum_{i=1}^{M}\sum_{j=1}^{M}\sum_{p=1}^{n}\sum_{q=1}^{n}\left\langle (\Delta\rho)^2\ \exp[-i\mathbf{q}\cdot(\mathbf{r}_{p,i}-\mathbf{r}_{q,j})]\right\rangle$$



assume spherical symmetry,
dilute mono-disperse ensemble

$$I(\mathbf{q}) \;=\; (\Delta\rho)^2\, nM^2 \cdot \underbrace{\frac{1}{M^2}\sum_{i,j}\left\langle \exp[-i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)]\right\rangle}\ \underbrace{\left[1 + \frac{1}{n}\sum_{p\neq q}\left\langle \exp[-i\mathbf{q}\cdot(\mathbf{r}_p-\mathbf{r}_q)]\right\rangle\right]}$$

intra particle correlations giving information on particle shape

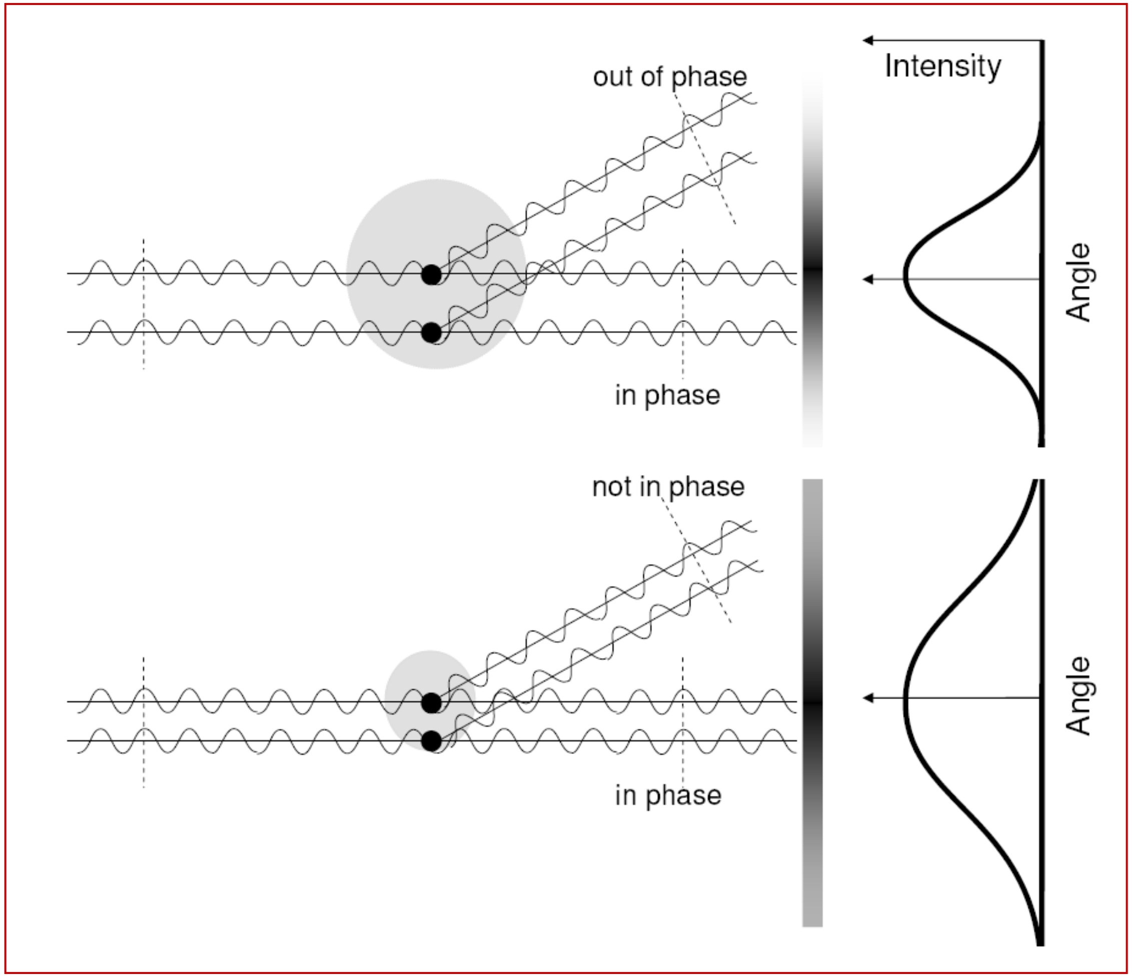
inter particle correlations approach 1 for dilute systems

$$I(\mathbf{q}) = (\Delta\rho)^2\, nM^2\, \boxed{P(\mathbf{q})}\, S(\mathbf{q})$$

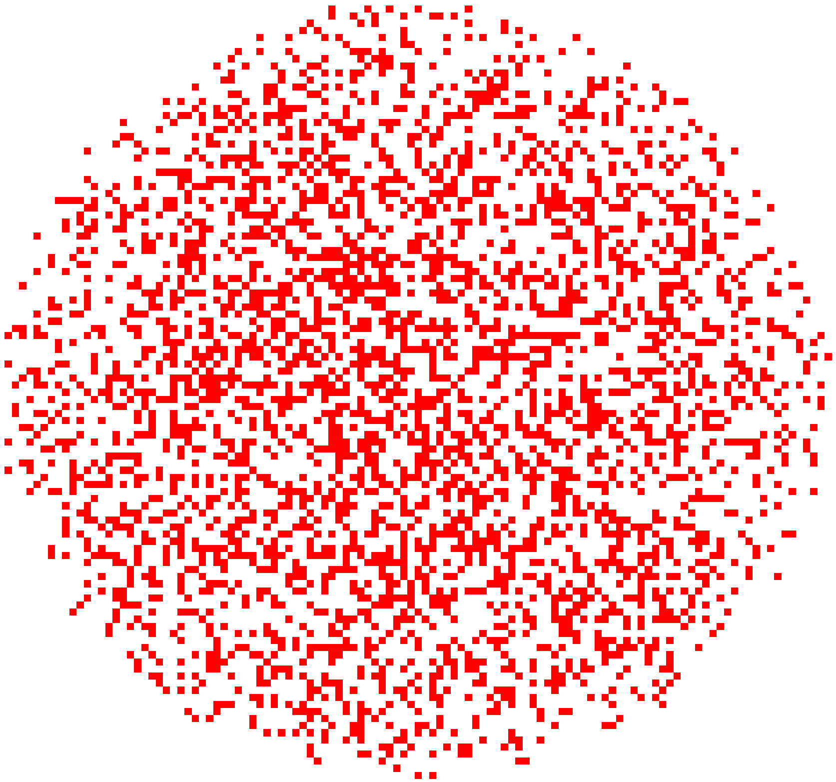
form factor

Form factor

$$P(\mathbf{q}) = \sum_i \sum_j \left\langle \exp[-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)] \right\rangle$$



Calculate the Form factor of sphere



http://bayesapp.org/simtest/

Calculation of small-angle scattering intensities ref

Name of a data file (optional): [ ] Browse...

Submit

Result is shown in a new window.

Subunits:

Form: [ ] Dimensions: [ ] [ ] [ ] Center: [ ] [ ] [ ] Rotation: [ ] [ ] Scattering length: [ ]

Form: [ ] Dimensions: [ ] [ ] [ ] Center: [ ] [ ] [ ] Rotation: [ ] [ ] Scattering length: [ ]

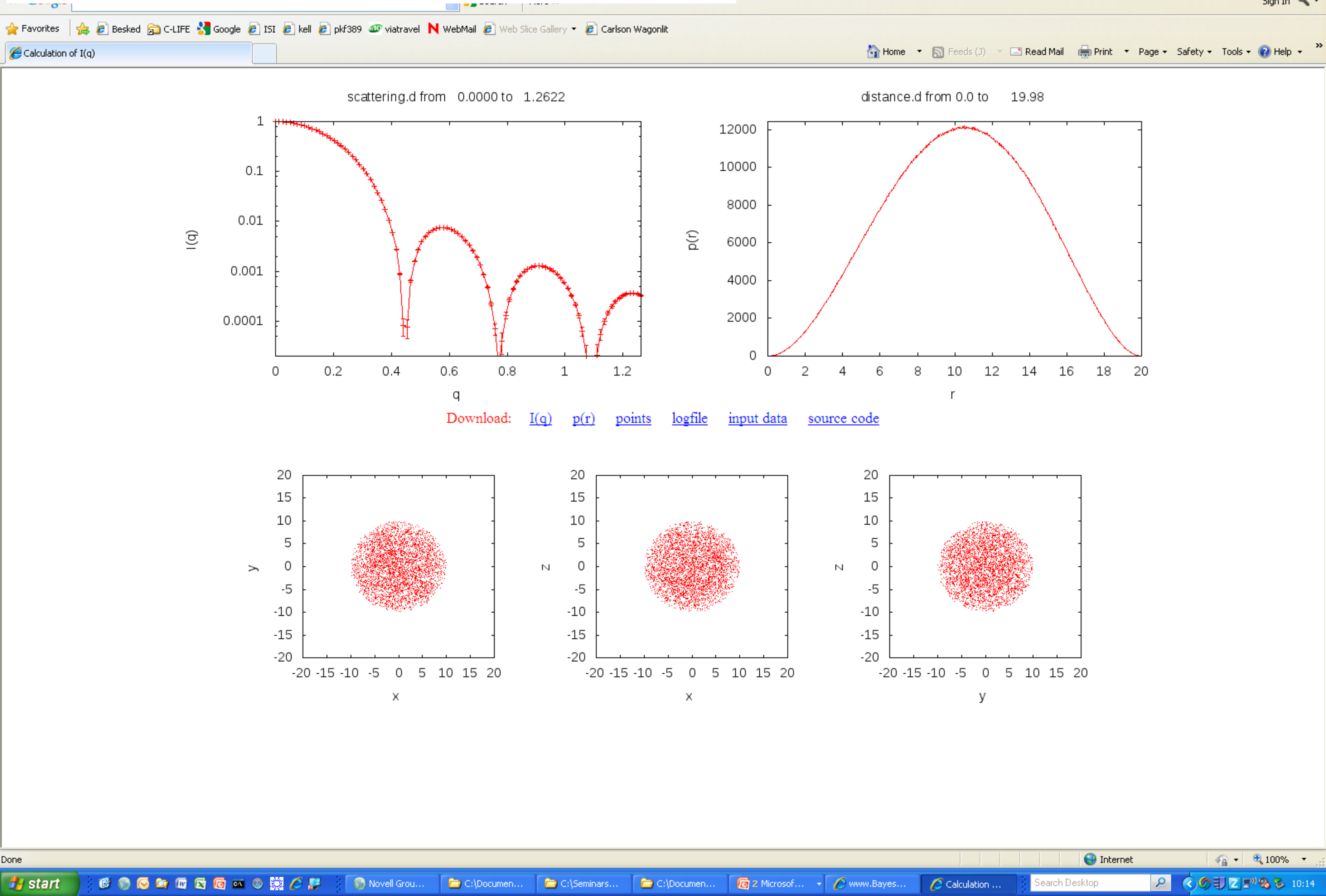
Form: [ ] Dimensions: [ ] [ ] [ ] Center: [ ] [ ] [ ] Rotation: [ ] [ ] Scattering length: [ ]

Form: [ ] Dimensions: [ ] [ ] [ ] Center: [ ] [ ] [ ] Rotation: [ ] [ ] Scattering length: [ ]

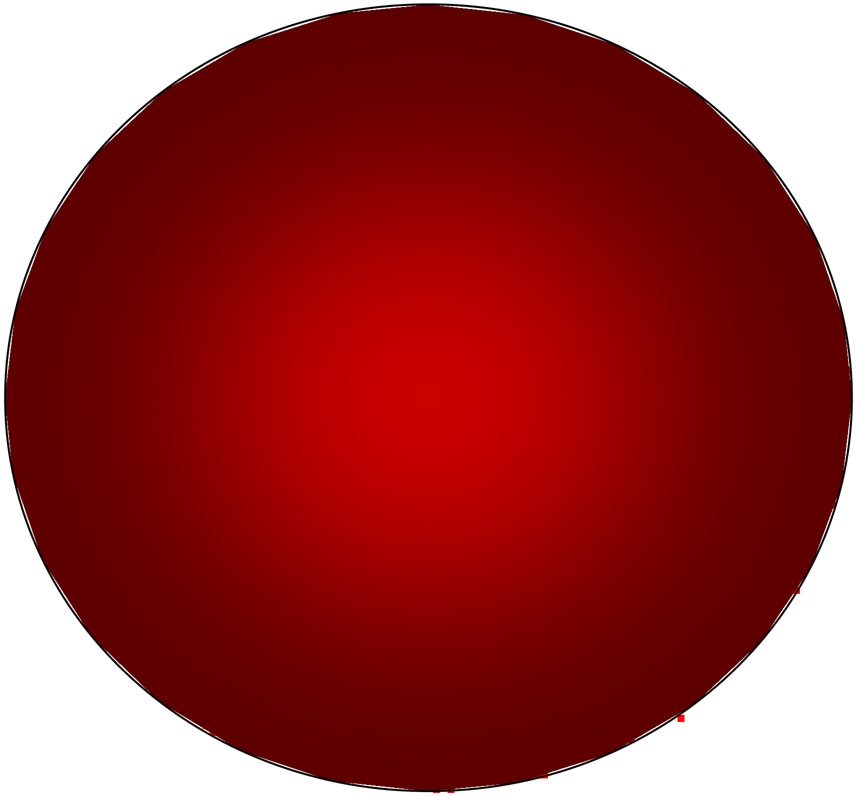
Form: [ ] Dimensions: [ ] [ ] [ ] Center: [ ] [ ] [ ] Rotation: [ ] [ ] Scattering length: [ ]

Steen Hansen slh@life.ku.dk.

http://bayesapp.org/sim/



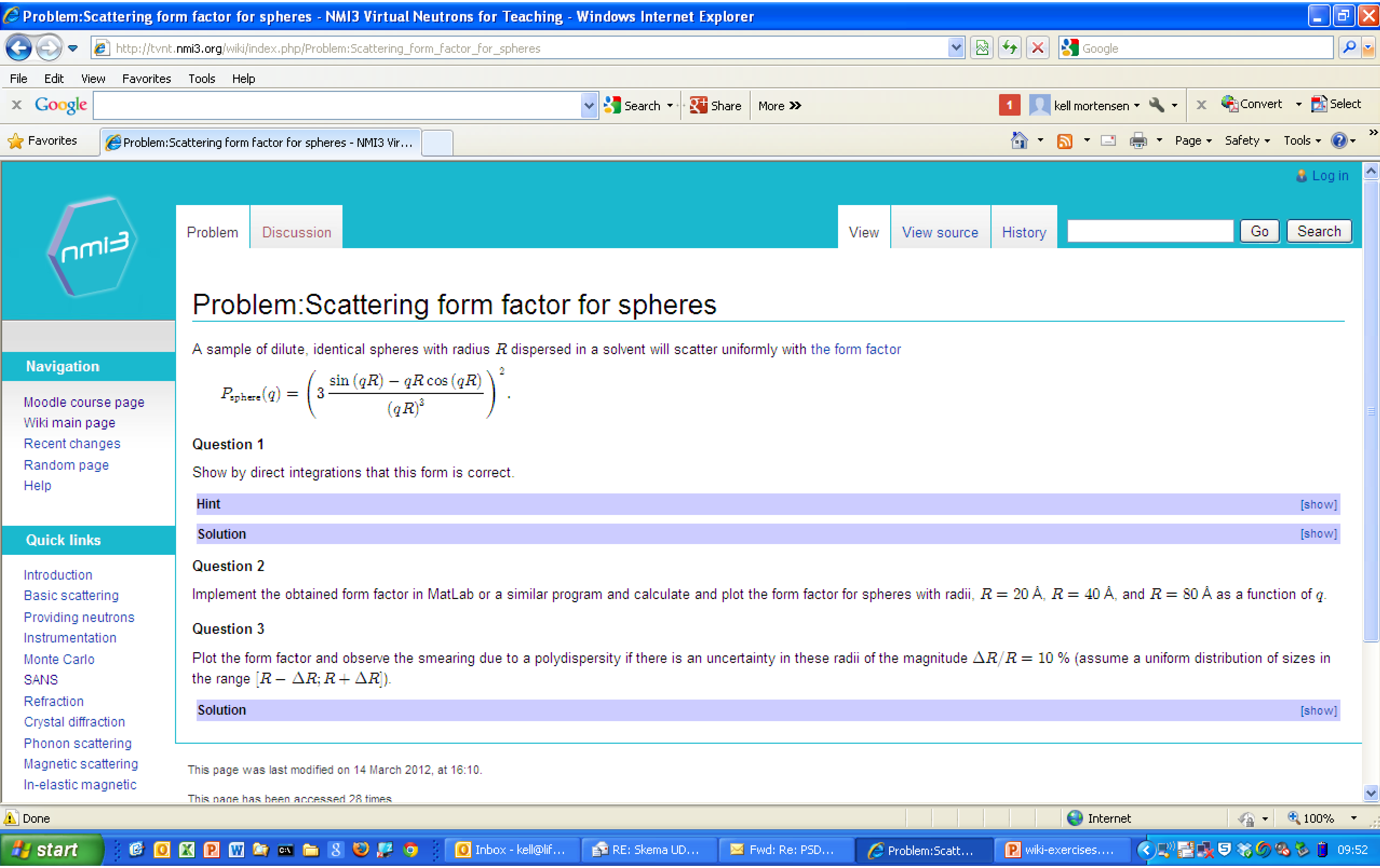
Calculate the Form factor of sphere



Analytical - Integral form

http://vnt.nmi3.org/wiki

http://vnt.nmi3.org/wiki/index.php/Problem:Scattering_form_factor_for_spheres



Problem:Scattering form factor for spheres - NMI3 Virtual Neutrons for Teaching - Windows Internet Explorer

Problem | Discussion | View | View source | History

Navigation
- Moodle course page
- Wiki main page
- Recent changes
- Random page
- Help

Quick links
- Introduction
- Basic scattering
- Providing neutrons
- Instrumentation
- Monte Carlo
- SANS
- Refraction
- Crystal diffraction
- Phonon scattering
- Magnetic scattering
- In-elastic magnetic

Problem:Scattering form factor for spheres

A sample of dilute, identical spheres with radius R dispersed in a solvent will scatter uniformly with the form factor

$$P_{\rm sphere}(q) = \left(3\,\frac{\sin(qR) - qR\cos(qR)}{(qR)^3}\right)^2 .$$

Question 1

Show by direct integrations that this form is correct.

Hint [show]

Solution [show]

Question 2

Implement the obtained form factor in MatLab or a similar program and calculate and plot the form factor for spheres with radii, $R = 20$ Å, $R = 40$ Å, and $R = 80$ Å as a function of q.

Question 3

Plot the form factor and observe the smearing due to a polydispersity if there is an uncertainty in these radii of the magnitude $\Delta R/R = 10$ % (assume a uniform distribution of sizes in the range $[R - \Delta R; R + \Delta R]$).

Solution [show]

This page was last modified on 14 March 2012, at 16:10.

This page has been accessed 28 times.

Problem:Scattering form factor for spheres

From NMI3 Virtual Neutrons for Teaching

A sample of dilute, identical spheres with radius R dispersed in a solvent will scatter uniformly with the form factor

$$P_{\mathrm{sphere}}(q) = \left(3\,\frac{\sin(qR) - qR\cos(qR)}{(qR)^3}\right)^2.$$

Hint [hide]

Use spherical coordinates or the Debye formula.

Problem:Scattering form factor for spheres

Solution [hide]

$V = 4\pi R^3/3$ and $\mathbf{q}\cdot\mathbf{r} = qr\cos(\theta)$. In spherical coordinates the volume element is $dV = r^2 \sin\theta \mathrm{d}r\mathrm{d}\theta\mathrm{d}\phi$.

$$\begin{aligned}
\frac{1}{V}\int \mathrm{dV} e^{-i\mathbf{q}\cdot\mathbf{r}} &= \frac{3}{4\pi R^3}\int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\int_0^{R}\mathrm{dr}\quad \mathrm{r}^2\sin\theta e^{-\mathrm{iqr}\cos\theta}\\
&= \frac{3}{2R^3}\int_0^{R}\mathrm{dr}\quad \mathrm{r}^2\int_{\cos\theta=-1}^{\cos\theta=1}\mathrm{d}(\cos\theta)e^{-\mathrm{iqr}\cos\theta}\\
&= \frac{3}{2R^3}\int_0^{R}\mathrm{dr}\quad \mathrm{r}^2\left(\frac{e^{-\mathrm{iqr}}-e^{\mathrm{iqr}}}{-\mathrm{iqr}}\right)\\
&= \frac{3}{R^3}\int_0^{R}\mathrm{dr}\quad \mathrm{r}^2\left(\frac{\sin(\mathrm{qr})}{\mathrm{qr}}\right)\\
&= \frac{3}{qR^3}\int_0^{R}\mathrm{dr}\quad \mathrm{r}\sin(\mathrm{qr})\\
&= \frac{3}{qR^3}\left[\frac{-r\cos(qr)}{q}\right]_0^R + \int_0^R \mathrm{dr}\quad \frac{\cos(\mathrm{qr})}{\mathrm{q}}\\
&= \frac{3}{qR^3}\left(\frac{-R\cos(qR)}{q}+\frac{\sin(qR)}{q^2}\right)\\
&= 3\frac{(\sin(qR)-qR\cos(qR))}{(qR)^3}.
\end{aligned}$$

Hence

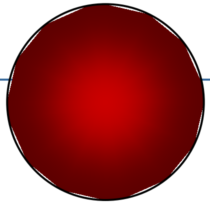
$$P_{\mathrm{sphere}}(q) = \left|\frac{1}{V}\int \mathrm{dV} e^{-i\mathbf{q}\cdot\mathbf{r}}\right|^2 = \left[\frac{(\sin qR - qR\cos qR)}{(qR)^3}\right]^2,$$

where $P \to 1$ for $q \to 0$.

The total intensity from a particle of volume $V[\text{Å}^3 = 10^{-24}\mathrm{cm}^3]$ in a solvent giving the excess scattering length $\Delta\rho\,[\mathrm{fm}/\text{Å}^3] = 0.1[\mathrm{cm}/\mathrm{cm}^3]$ is

$$I(q) = \phi V(\Delta\rho)^2 P.$$

Calculate the Form factor of sphere



Use, that the scattering amplitude from a homogeneous volume V can be written

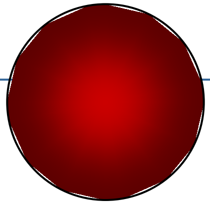
$$A(\mathbf{q}) = \frac{1}{V}\int_{sphere} \rho(\mathbf{r}) \exp[-i\mathbf{q}\cdot\mathbf{r}] d\mathbf{r}$$

to calculate the form factor P(q)
of a homogeneous sphere of radius R.

You may need the integral formula

$$\int x \sin x dx = \sin x - x\cos x$$

Form factor of sphere



Sphere

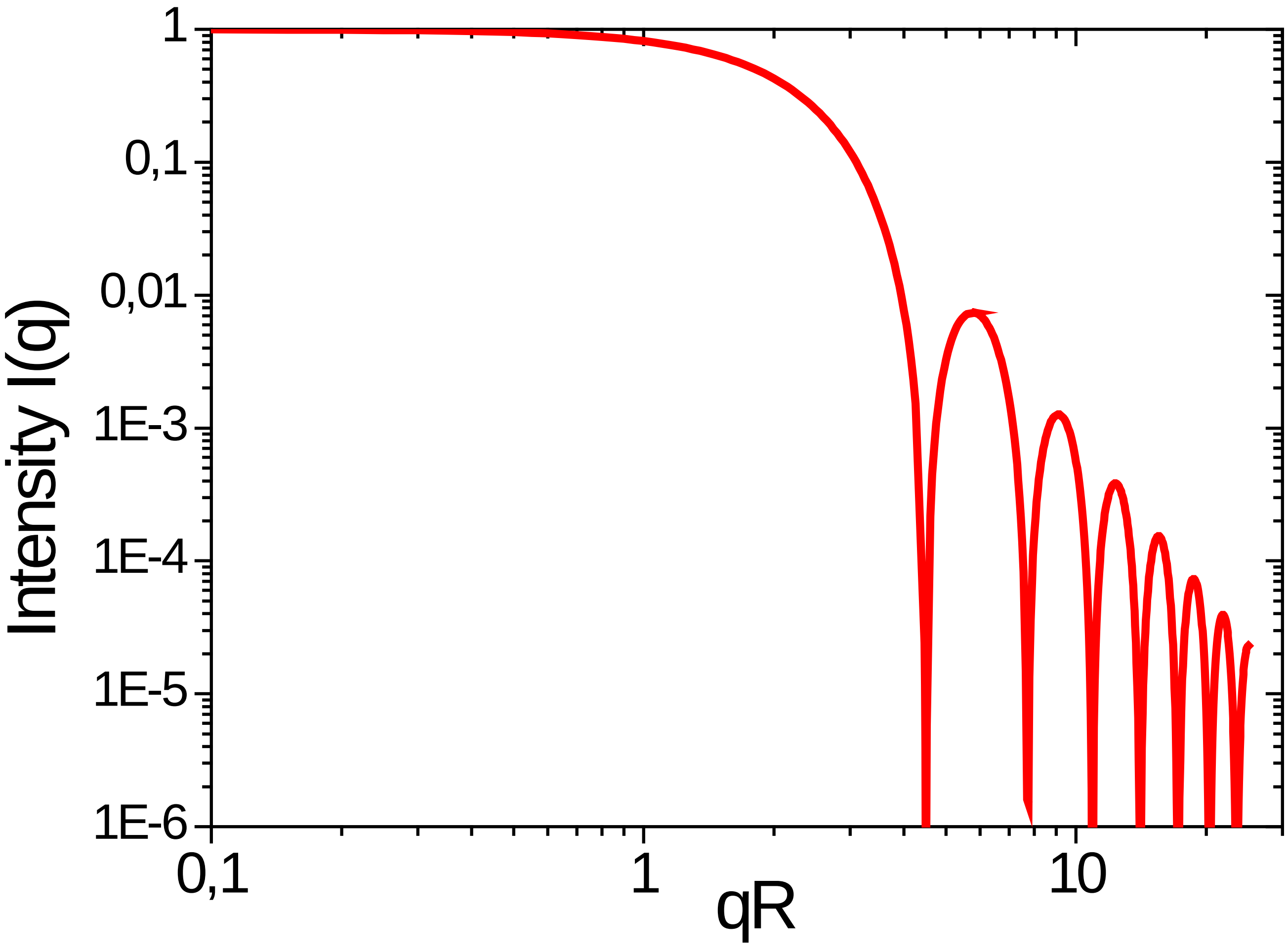
$$\boxed{A(\mathbf{q}) = \frac{1}{V}\int_{sphere} \rho(\mathbf{r}) \exp[-i\mathbf{q}\cdot\mathbf{r}]d\mathbf{r}}$$

$$\boxed{\mathbf{q}\cdot\mathbf{r} = q\ r\ \ \cos(\theta) = q\ r\ u, \qquad u = \cos(\theta)}$$

$$\begin{aligned}
A(\mathbf{q}) &= \frac{1}{V}\int_V \exp[-i\mathbf{q}\cdot\mathbf{r}]d\mathbf{r} \\
&= \frac{1}{V}\int_\phi\int_\theta\int_r \exp[-iqr\cos\theta]\ r^2dr\ \ \sin\theta d\theta\ d\phi \\
&= \frac{2\pi}{V}\int_{u=-1}^{1}\int_{r=0}^{R} \exp[-iqru]\ r^2dr\ du \\
&= \frac{2\pi}{V}\int_{u=-1}^{1}\int_{r=0}^{R} [\cos(qru) - i\sin(qru)]\ r^2dr\ du \\
&= \frac{2\pi}{V}\left[\int_{r=0}^{R}[\sin(qru) + i\cos(qru)]\ r^2dr\right]_{u=-1}^{1} \\
&= \frac{2\pi}{V}\left[\int_{r=0}^{R}\frac{2}{qr}\sin(qr)\ r^2dr\right]_{u=-1}^{1} \\
&= \frac{4\pi}{V}\frac{1}{q^3}\int_{x=0}^{qR}\sin x x dx \\
&= \frac{4\pi}{V}\frac{1}{q^3}\Big[\sin x - x\cos x\Big]_{x=0}^{qR} \\
&= \frac{3}{(qR)^3}[\sin(qR) - qR\cos(qR)]
\end{aligned}$$

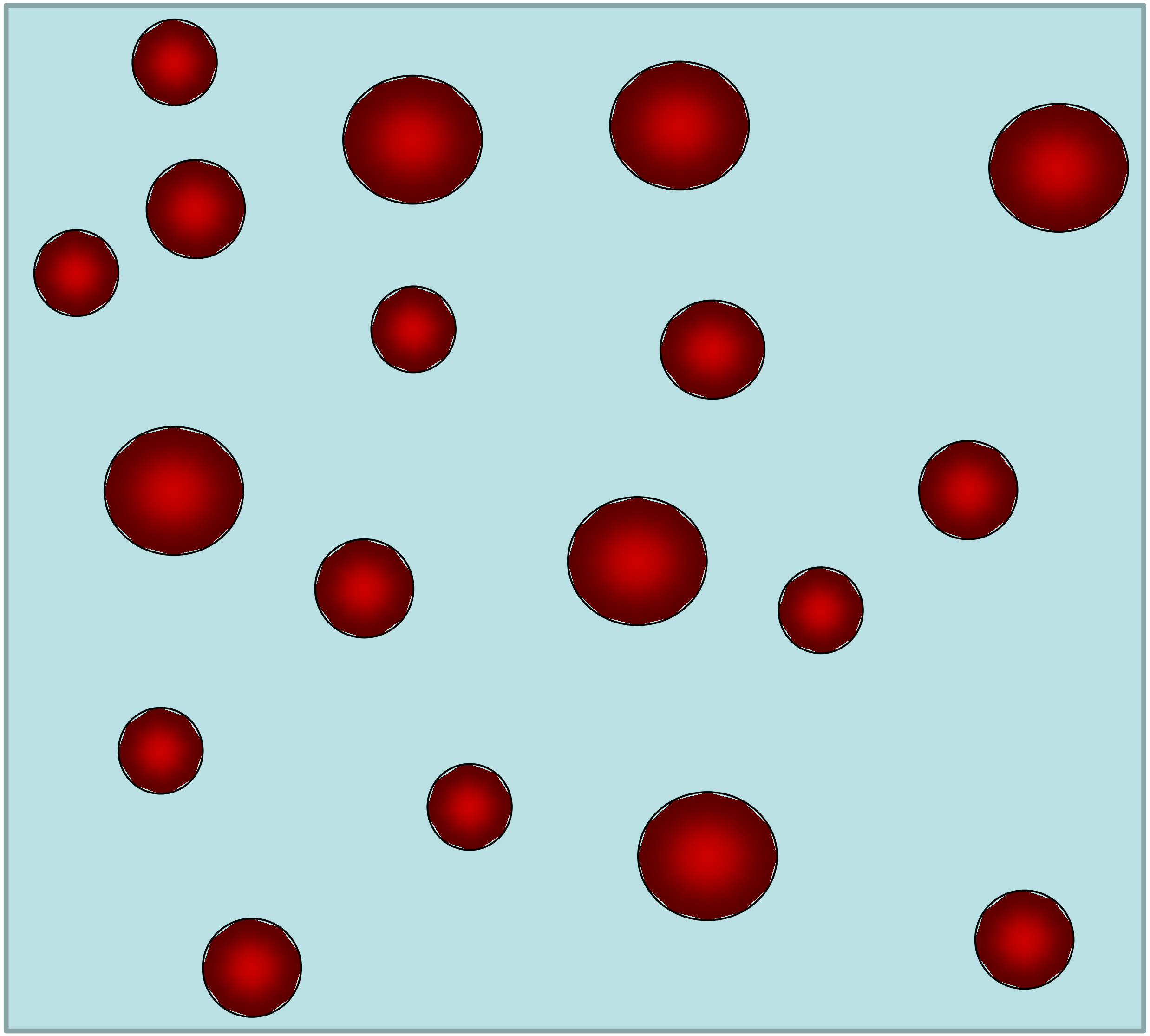
$$\boxed{\int x\sin x dx = \sin x - x\cos x}$$

$$\boxed{P(q) = A^2(q) = \left[\frac{3}{(qR)^3}[\sin(qR) - qR\cos(qR)]\right]^2}$$



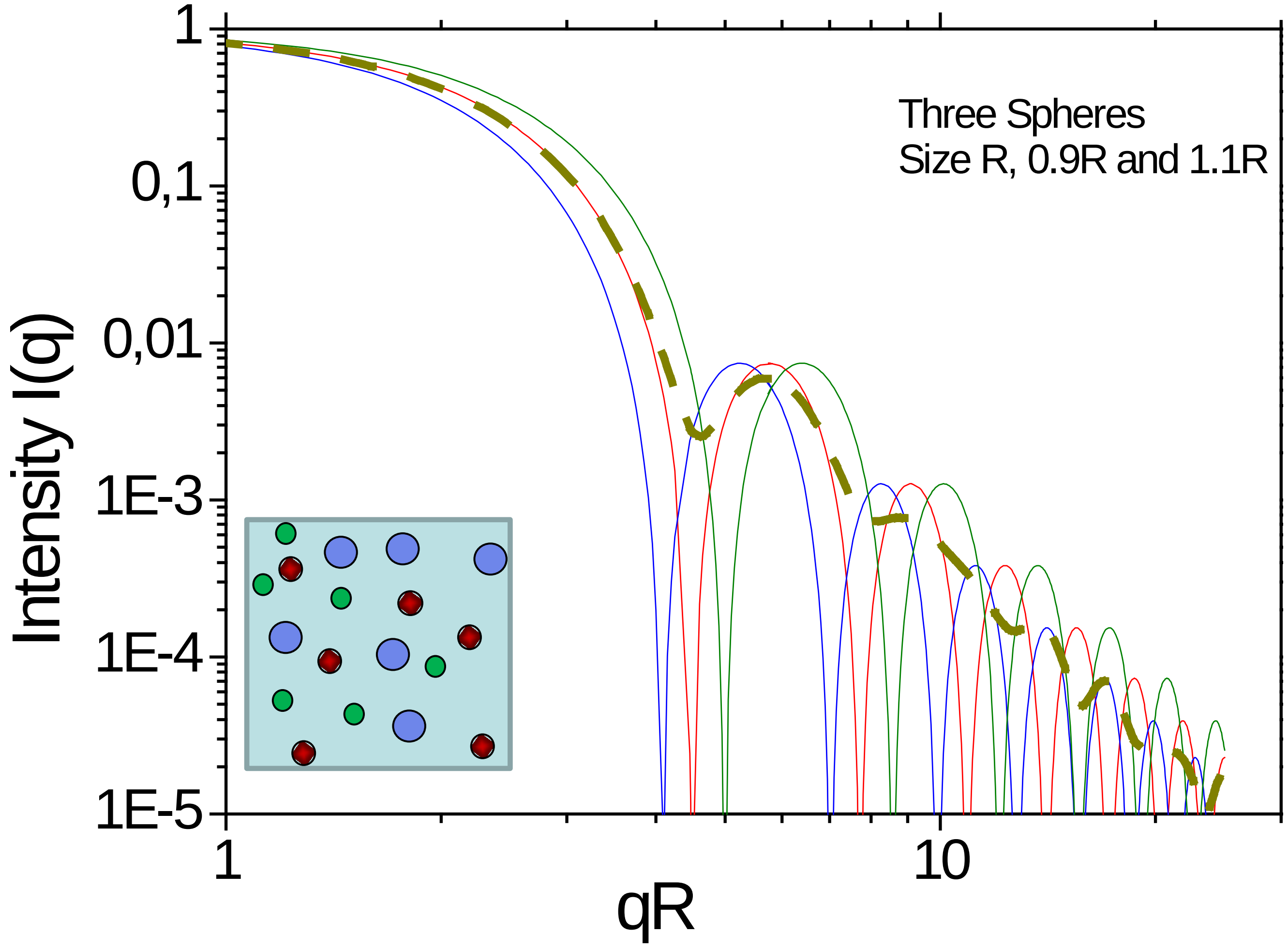
$$P(q) = A^2(q) = \left[\frac{3}{(qR)^3}[\sin(qR) - qR\cos(qR)]\right]^2$$

Polydispercity



Polydispercity

$$I(q) = [\Delta\rho_1]^2 n_1 M_1^2\, P(q,R_1) + [\Delta\rho_2]^2 n_2 M_2^2\, P(q,R_2) + [\Delta\rho_3]^2 n_3 M_3^2\, P(q,R_3)$$

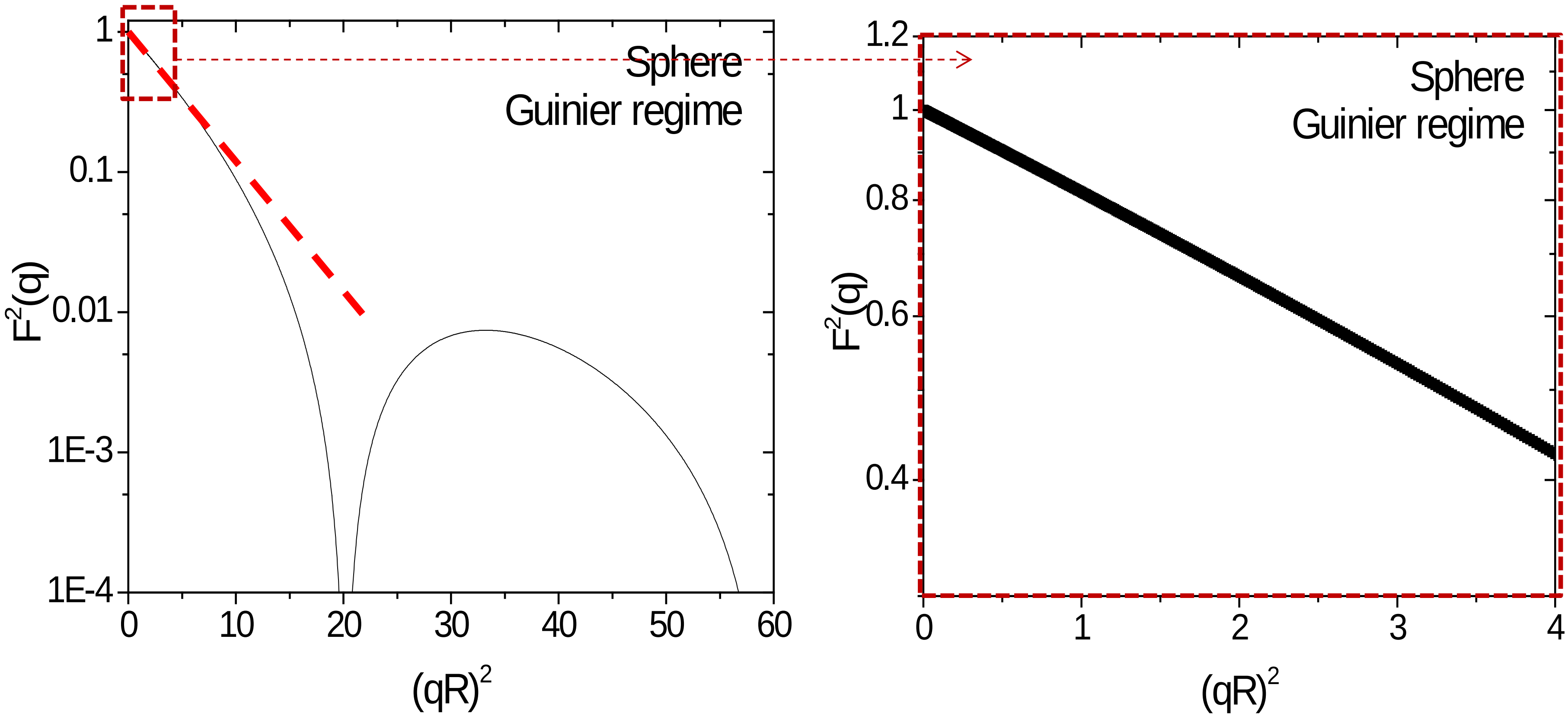


Guinier Approximation

Low-q approximation for the sphere

Formfactor of a sphere with radius R

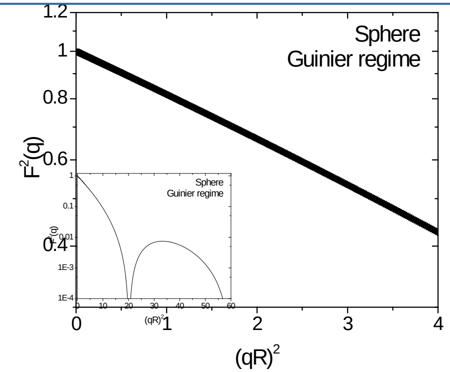
$$P(q) = \left[\frac{3}{(qR)^3}[\sin(qR) \; - \; qR\cos(qR)]^3\right]^2$$



Low-q approximation for the sphere

Low-q regime

$$P(q) = \left[\frac{3}{(qR)^3} [\sin(qR) \;-\; qR\cos(qR)]^3 \right]^2$$



Use Taylor expansion

$$f(x) \approx f(0) + x * f'(0) + \frac{1}{2}x^2 f''(0) + \frac{1}{3!}x^3 f'''(0) + \frac{1}{4!}x^4 f''''(0) + \frac{1}{5!}x^5 f'''''(0) + \ldots$$

which on the sin- and cos-functions – to 5th order in x - gives

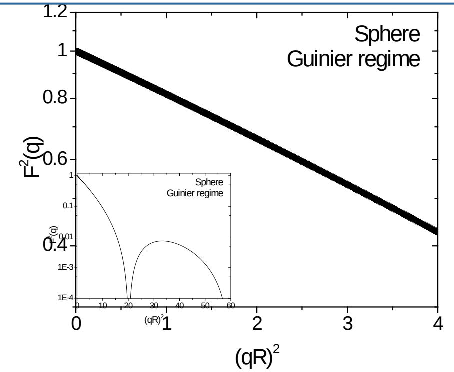
$$\begin{aligned} \sin(x) &\approx \sin 0 + x\cos 0 - \frac{1}{2}x^2 \sin 0 - \frac{1}{6}x^3 \cos 0 + \frac{1}{24}x^4 sin0 - \frac{1}{120}x^5 cos0 \\ &= x - \frac{1}{6}x^3 + \frac{1}{120}x^5 \end{aligned}$$

$$\begin{aligned} \cos(x) &\approx \cos 0 - x\sin 0 - \frac{1}{2}x^2 \cos 0 + \frac{1}{6}x^3 \sin 0 + \frac{1}{24}x^4 cos0 \\ &= 1 - \frac{1}{2}x^2 + \frac{1}{24}x^4 \end{aligned}$$

Low-q approximation for the sphere

Low-q regime

$$P(q) = \left[\frac{3}{(qR)^3}[\sin(qR) \;-\; qR\cos(qR)]^3\right]^2$$



From the Taylor expansions we then have

$$\begin{aligned}\sin(x) - x\cos(x) &\approx (x - \frac{1}{6}x^3 + \frac{1}{120}x^5) - x(1 - \frac{1}{2}x^2 + \frac{1}{24}x^4) \\ &= \frac{1}{3}x^3 - \frac{1}{30}x^5\end{aligned}$$

and thereby the amplitude of scattering

$$F_{sphere}(x) = 3\,\frac{\sin(x) - x\cos(x)}{x^3} = 1 - \frac{1}{10}x^2 \qquad x = qR$$

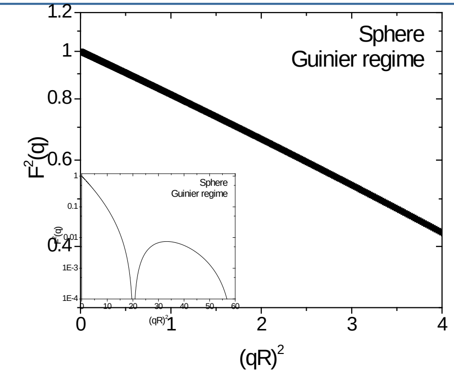
The form factor of spheres is then approached

$$P(q) = F^2(q) = (1 - \frac{1}{10}x^2)^2 \approx 1 - \frac{1}{5}x^2 \approx \exp[-\frac{1}{5}x^2]$$

Guinier approximation

Low-*q* regime

$$P(q) = \left[\frac{3}{(qR)^3}[\sin(qR) \;-\; qR\cos(qR)]^3\right]^2$$



From the Taylor expansions we then have

$$P(q) \approx \exp[-\frac{1}{5}q^2R^2]$$

More generally, it can be shown that the linear

$$\ln(P) \;\sim\; q^2$$

relationship holds for all systems of spherical symmetry, as described by the radius of gyration R_g

$$P(q) \approx \exp[-\frac{1}{3}q^2R_g^2]$$

The radius of a sphere is therefore related to the radius of gyration as

$$\boxed{R_g^2 = \frac{3}{5}R^2}$$

Guinier approximation

$$I(\mathbf{q}) = V \int \langle \rho(\mathbf{r}' - \mathbf{r})\rho(\mathbf{r}') \rangle \ \exp(-i\mathbf{q} \cdot \mathbf{r}) \ d\mathbf{r}$$

which in spherical symmetric case become:

$$\begin{aligned} I(q) &= V \int \langle \rho(r' - r)\rho(r') \rangle \ r^2 \ \frac{\sin(qr)}{qr} \ dr \\ &\propto V \int \langle \gamma(r) \rangle \ r \ \frac{sin(qr)}{qr} \ dr \end{aligned}$$

for small qr-values:

$$\frac{\sin(qr)}{qr} = 1 - \frac{1}{3!}(rq)^2 + \dots$$

giving:

$$\begin{aligned} I(q) &\propto V \int \gamma(r) r^2 \ dr - \frac{1}{3} \cdot \frac{1}{2} \int \gamma(r) r^4 q^4 dr + \dots \\ &= V \int \gamma(r) r^2 \ dr \ (\ 1 - \frac{1}{3} q^2 \cdot \boxed{\frac{1}{2} \frac{\int \gamma(r) r^4 dr}{\int \gamma(r) r^2 \ dr}} + \dots) \\ &= V \int \gamma(r) r^2 \ dr \ (\ 1 - \frac{1}{3} R_g^2 q^2 + \dots) \end{aligned}$$

Guinier Approximation

$$I(q) \propto V\int \gamma(r)r^2\,dr - \frac{1}{3}\cdot\frac{1}{2}\int \gamma(r)r^4q^4dr + \ldots$$
$$= V\int \gamma(r)r^2\,dr\,\left(1 - \frac{1}{3}q^2\cdot \boxed{\frac{1}{2}\frac{\int\gamma(r)r^4dr}{\int\gamma(r)r^2\,dr}} + \ldots\right)$$
$$= V\int \gamma(r)r^2\,dr\,\left(1 - \frac{1}{3}R_g^2q^2 + \ldots\right)$$

and thus with $\exp(x) \sim 1 + x + \ldots$

$$\boxed{I(q) = \exp(-R_g^2q^2/3)}$$

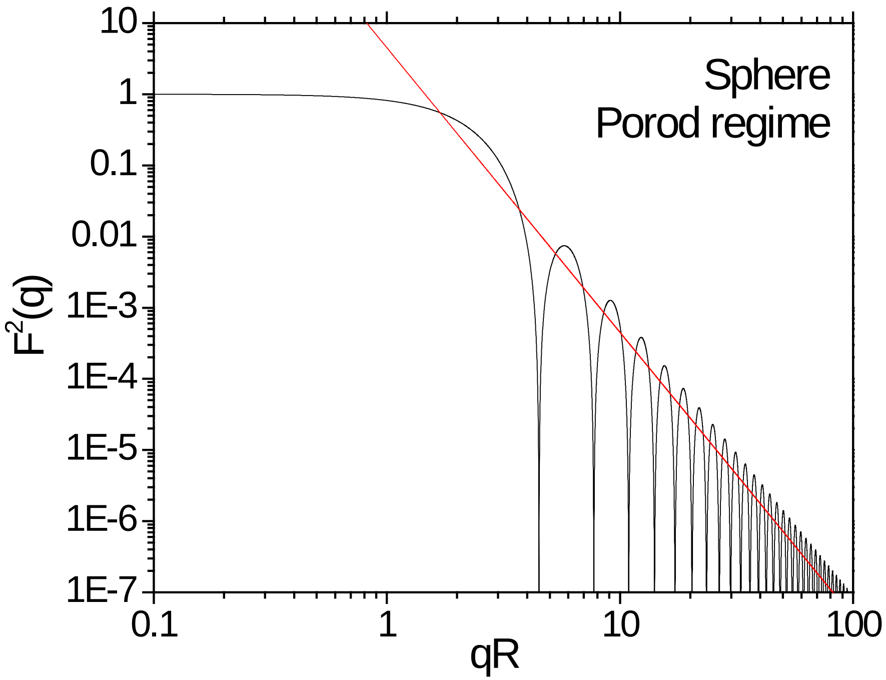
independent of particle form,
but valid range depend on particular form

High-q limit
POROD REGIME

Porod Law for a sphere

Amplitude $F(q)$ squared

$$
\begin{aligned}
F^2(q) &= 9V^2 \left[\frac{\sin(qR) - qR\cos(qR)}{(qR)^3}\right]^2 \\
&= 9V^2 \left[\frac{\sin(qR)}{qR} - \cos(qR)\right]^2 \cdot (qR)^{-4} \\
&\to 9V^2 \cos^2(qR) \cdot (qR)^{-4} \quad \text{for } qR \to \infty
\end{aligned}
$$



Averaging over the cosine oscillations, we have for

$$qR \to \infty$$

$$
\begin{aligned}
F^2(q) &\to 9V^2 \langle\cos^2(qR)\rangle \cdot (qR)^{-4} \\
&= 9V^2/2 \cdot (qR)^{-4}
\end{aligned}
$$

and thereby

$$\boxed{F^2(q) \to \frac{9}{2}V^2 \cdot (qR)^{-4} = 2\pi A \cdot q^{-4}}$$

$A(R)$ being the surface area of the sphere

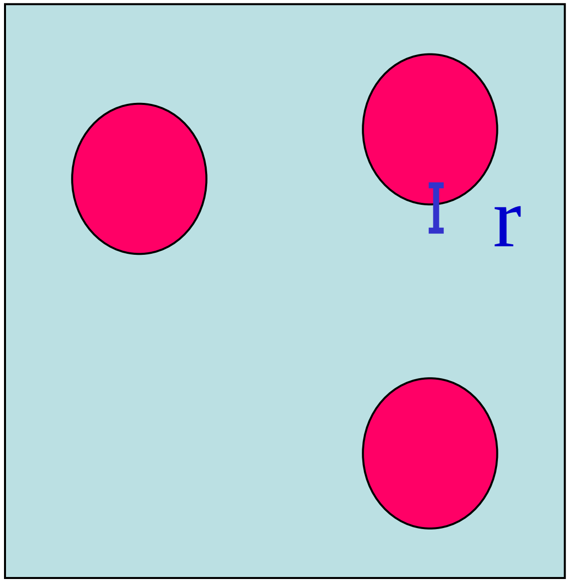
Porod Law - for two phase system

In the small r-regime (large q-regime)
the scattering can only depend on interfase properties.
In this small r-regime, $\gamma(r)$ can be Taylor expanded

$$\gamma(r) \propto 1 + a_1 r + a_2 r^2 + \ldots$$

Porod showed, that for a simple two-phase system, we have to first order in r

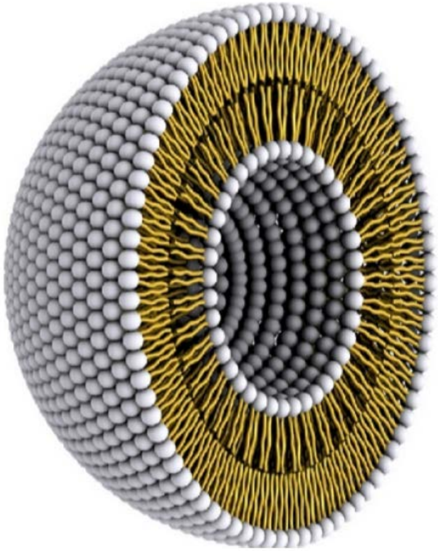
$$\gamma(r) \propto 1 - \frac{S}{4V} r$$



Giving the Porod Law

$$\begin{aligned} I(q) &\sim \int \gamma(r) \frac{\sin(qr)}{qr}\, dr \\ &\sim \int (1 - \frac{S}{4V} r) \frac{\sin(qr)}{qr} dr \\ &\sim \frac{S}{V} \boxed{q^{-4}} \end{aligned}$$

Spherical Shells
(Micelles and Liposomes)

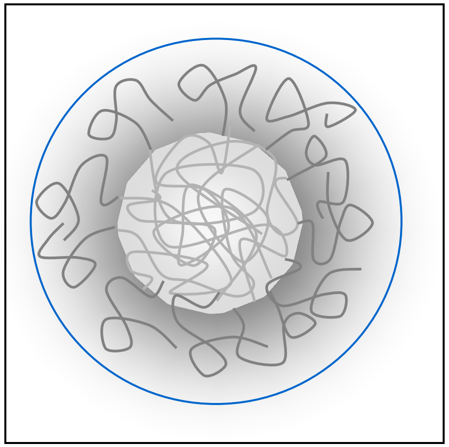


Form factor of Micelle modeled as Core - Shell Structure

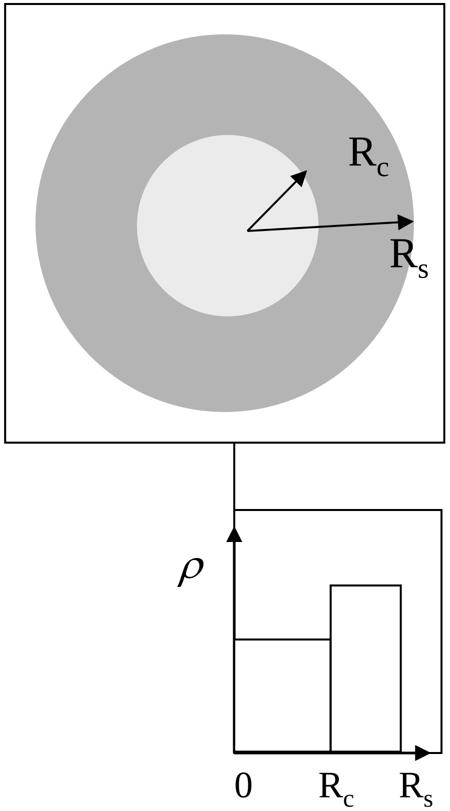
Form Factor Amplitude

$$A(q) = \int \rho(r) \frac{\sin(qr)}{qr}\, r^2\, dr$$

Core-Shell particle:

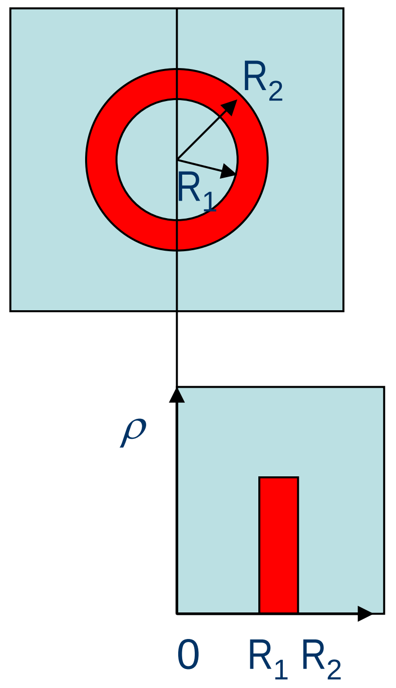


$$A_{\rm cs}(q) = \int_0^{R_c} \Delta\rho_c \frac{\sin(qr)}{qr}\, r^2\, dr + \int_{R_c}^{R_s} \Delta\rho_s \frac{\sin(qr)}{qr}\, r^2\, dr$$



$$\begin{aligned}
A_{\rm cs}(q) &= \Delta\rho_c \int_0^{R_c} \frac{\sin(qr)}{qr}\, r^2\, dr \\
&\quad + \left(\Delta\rho_s \int_0^{R_s} \frac{\sin(qr)}{qr}\, r^2\, dr - \Delta\rho_s \int_0^{R_c} \frac{\sin(qr)}{qr}\, r^2\, dr \right) \\
&= (\Delta\rho_c - \Delta\rho_s) \int_0^{R_c} \frac{\sin(qr)}{qr}\, r^2\, dr + \Delta\rho_s \int_0^{R_s} \frac{\sin(qr)}{qr}\, r^2\, dr \\
&= \frac{(\rho_c - \rho_s) R_c^3 A_{\rm sp}(q, R_c) + \Delta\rho_s R_s^3 A_{\rm sp}((q, R_s)}{(\rho_c - \rho_s) R_c^3 + \Delta\rho_s R_s^3}
\end{aligned}$$

Form factor of Spherical Shell Structure



Amplitude

$$\begin{aligned} A_{\mathrm{cs}}(q) &= \Delta\rho_c \int_0^{R_c} \frac{\sin(qr)}{qr}\, r^2\, dr \\ &\quad + \left(\Delta\rho_s \int_0^{R_s} \frac{\sin(qr)}{qr}\, r^2\, dr - \Delta\rho_s \int_0^{R_c} \frac{\sin(qr)}{qr}\, r^2\, dr \right) \\ &= (\Delta\rho_c - \Delta\rho_s) \int_0^{R_c} \frac{\sin(qr)}{qr}\, r^2\, dr + \Delta\rho_s \int_0^{R_s} \frac{\sin(qr)}{qr}\, r^2\, dr \\ &= \frac{(\rho_c - \rho_s) R_c^3 A_{\mathrm{sp}}(q, R_c) + \Delta\rho_s R_s^3 A_{\mathrm{sp}}((q, R_s)}{(\rho_c - \rho_s) R_c^3 + \Delta\rho_s R_s^3} \end{aligned}$$

Shell: $\Delta\rho_c = 0$

Giving,

$$A_s(q) = \frac{(\Delta\rho_s)\left(R_c^3 A_s(q, R_c) + R_s^3 A_s((q, R_s) \right)}{(\Delta\rho_s)(R_c^3 + R_s^3)}$$

Calculation of small-angle scattering intensities from a model of subunits ref

Name of a data file for comparison (optional): Browse...

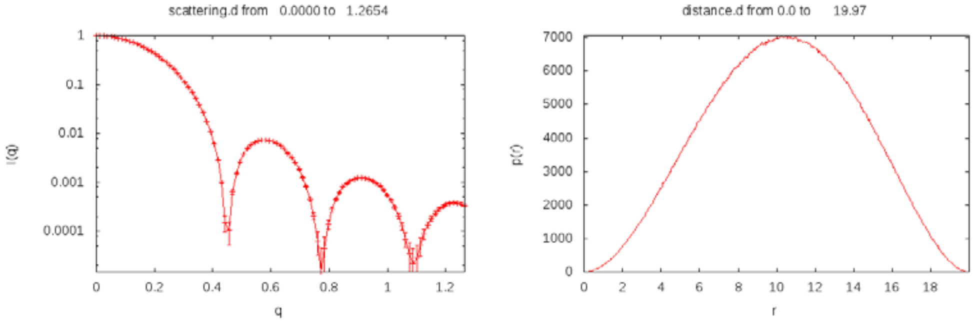
Submit Result is shown in a new window.

Subunits:

The model of the scatterer can be composed of several subunits to be defined below.
Overlapping subvolumes are automatically subtracted as described in the reference,
unless the letter X is entered in the following box: X
A total of 15000 points are used in this webversion of the program.
For a more detailed calculation the source code can be downloaded.
To start the calculation press "enter" on the keyboard when the cursor is in an input field or press the "Submit"-button above.

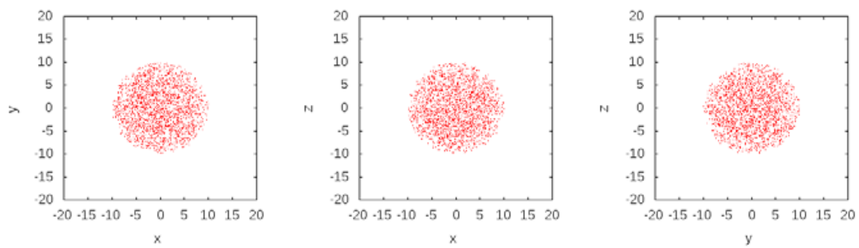
Form:	Dimensions:			Center:			Rotation:		Scattering length:
s	10								1
s	9								-1

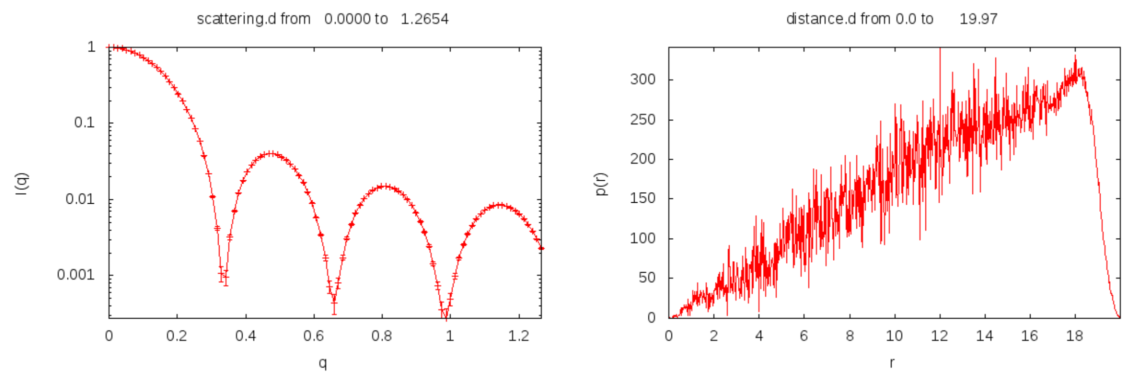
Noise: No points: Qmin: Qmax: Rel: Abs: Smear: **Vol. fraction:** **Polydisperse:**



Sphere
Radius 10

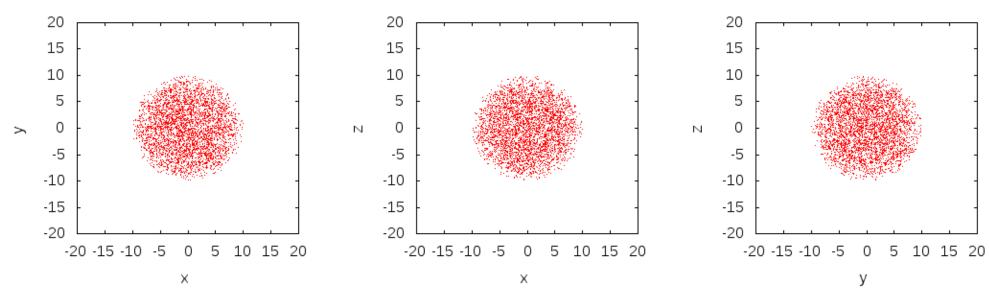
Download: I(q) P(q) p(r) points logfile input data noise data source code





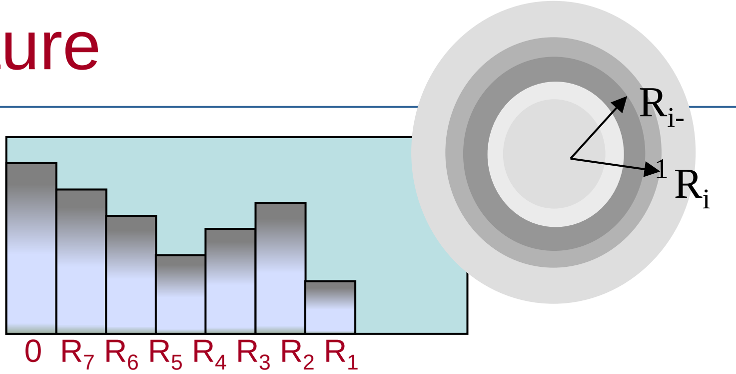
Download: I(q) P(q) p(r) points logfile input data noise data source code

Shell
Radius 10
Thickness 1



Kell Mortensen

Form factor of Spherical Shell Structure



Amplitude

$$
\begin{aligned}
F(q) &= \int_0^\infty \rho(r)\frac{\sin(qr)}{qr}\,4\pi r^2\,dr \\
&= \int_0^{R_1} \rho_1\frac{\sin(qr)}{qr}\,4\pi r^2\,dr + \int_{R_1}^{R_2} \rho_2\frac{\sin(qr)}{qr}\,4\pi r^2\,dr \quad ++ \\
&= \int_0^{R_1} \rho_1\frac{\sin(qr)}{qr}\,4\pi r^2\,dr + \left[\int_0^{R_2} \rho_2\frac{\sin(qr)}{qr}\,4\pi r^2\,dr - \int_0^{R_1} \rho_2\frac{\sin(qr)}{qr}\,4\pi r^2\,dr\right] \quad ++
\end{aligned}
$$

giving, as in the calculation for a dense sphere

$$
F(q) = \frac{1}{\mathcal{V}}\left[\rho_1 V(R_1)F_s(q,R_1) + \sum_{i=2}^{N}\rho_i\Big(V(R_\mathrm{i})F_s(q,R_\mathrm{i}) - V(R_{\mathrm{i}-1})F_s(q,R_{\mathrm{i}-1})\Big)\right]
$$

where

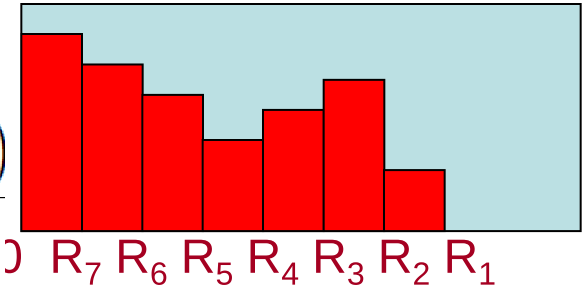
$$
\mathcal{V} = \rho_1 V(R_1) + \sum_{i=2}^{N}\rho_\mathrm{i}\Big(V(R_\mathrm{i}) - V(R_{\mathrm{i}-1})\Big)
$$

if we define $\rho_o = 0$ and $R_0 = 0$ the equation can be generalized to

$$
F(q) = \frac{\sum_{i=1}^{N}\rho_i\Big(V(R_\mathrm{i})F_s(q,R_\mathrm{i}) - V(R_{\mathrm{i}-1})F_s(q,R_{\mathrm{i}-1})\Big)}{\sum_{i=1}^{N}\rho_\mathrm{i}\Big(V(R_\mathrm{i}) - V(R_{\mathrm{i}-1})\Big)}
$$

Form factor of Spherical Shell Structure

Amplitude



$$F(q) \quad = \quad \frac{\sum_{i=1}^{N} \rho_i \Big(V(R_{\mathrm{i}}) F_s(q, R_{\mathrm{i}}) - V(R_{\mathrm{i}-1}) F_s(q, R_{\mathrm{i}-1}) \Big)}{\sum_{i=1}^{N} \rho_{\mathrm{i}} \Big(V(R_{\mathrm{i}}) - V(R_{\mathrm{i}-1}) \Big)}$$

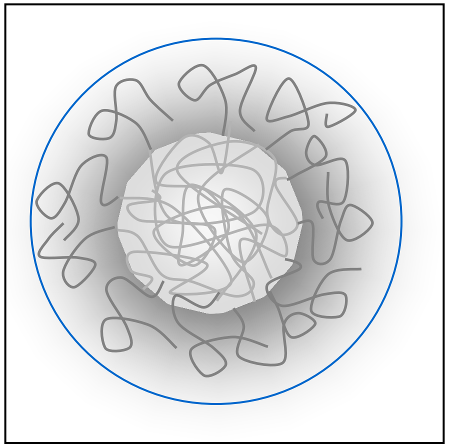
Inset expression for spherical form factor:

$$F(q) \quad = \quad \frac{3 \sum_{\mathrm{i}=1}^{N} \rho_{\mathrm{i}} \Big[\Big(\sin(qR_{\mathrm{i}}) - qR_{\mathrm{i}} \cos(qR_{\mathrm{i}}) \Big) - \Big(\sin(qR_{\mathrm{i}-1}) - qR_{\mathrm{i}-1} \cos(qR_{\mathrm{i}-1}) \Big) \Big]}{\sum_{\mathrm{i}=1}^{N} (\rho_{\mathrm{i}} \Big[(qR_{\mathrm{i}})^3 - (qR_{\mathrm{i}-1})^3 \Big]}$$

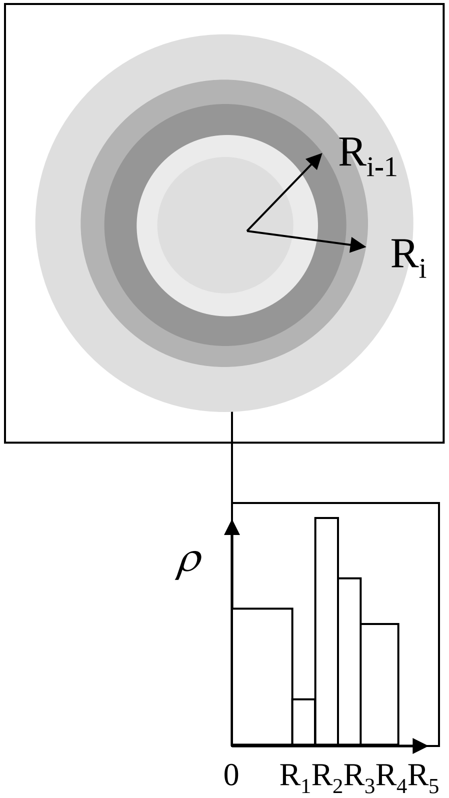
and thereby the scattering intensity

$$\boxed{I(q) = F^2(q) = \left[\frac{3 \sum_{\mathrm{i}=1}^{N} \rho_{\mathrm{i}} \Big[\Big(\sin(qR_{\mathrm{i}}) - qR_{\mathrm{i}} \cos(qR_{\mathrm{i}}) \Big) - \Big(\sin(qR_{\mathrm{i}-1}) - qR_{\mathrm{i}-1} \cos(qR_{\mathrm{i}-1}) \Big) \Big]}{\sum_{\mathrm{i}=1}^{N} (\rho_{\mathrm{i}} \Big[(qR_{\mathrm{i}})^3 - (qR_{\mathrm{i}-1})^3 \Big]} \right]^2}$$

Form factor of Micelle modeled as Spherical Shell Structure

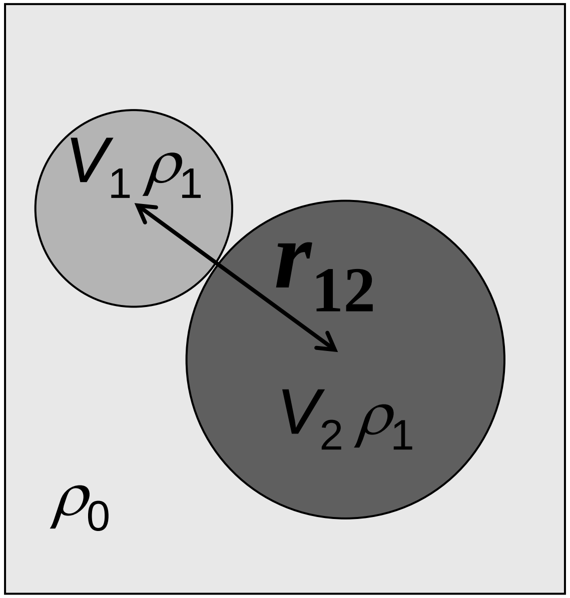


COMPOUND PARTICLE build up of sub-units (concentric spheres / shells)

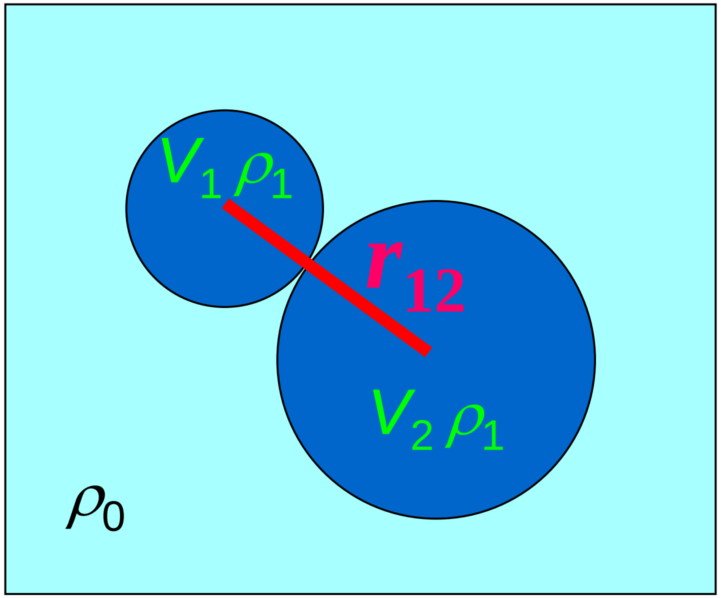


Form factor of Particle modeled as Two Spheres

COMPOUND PARTICLE
build up of sub-units
(concentric spheres / shells)



Compound particles:



examples:
nucleosomes, protein/DNA complexes
ribosomes: protein/RNA complexes

$$I(\mathbf{q}) = \int_V \int_V \langle \delta\rho(\mathbf{r})\ \delta\rho(\mathbf{r}')\rangle e^{-i\mathbf{q}\cdot\mathbf{r}}\ d\mathbf{r}d\mathbf{r}'$$
$$= \left\langle \left| \int_V \delta\rho(\mathbf{r})\ e^{-i\mathbf{q}\cdot\mathbf{r}}\ d\mathbf{r}d\mathbf{r}' \right|^2 \right\rangle$$

With $V = V_1 + V_2$

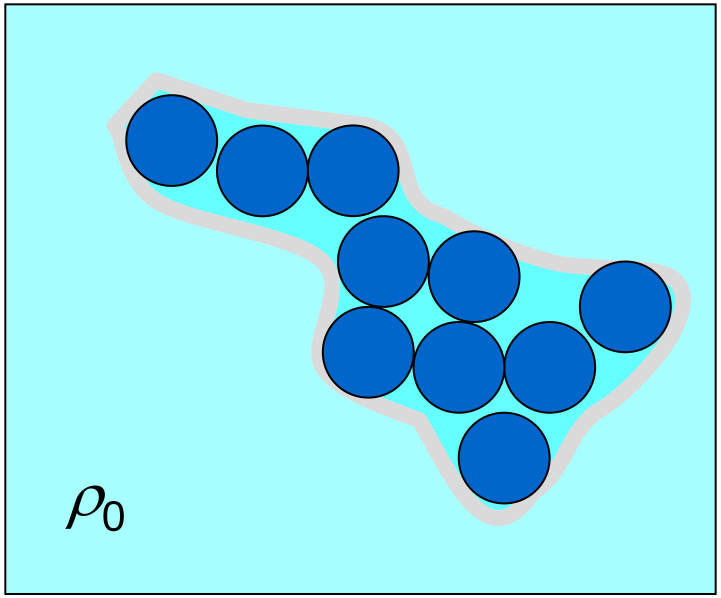
$$I(\mathbf{q}) = \left\langle \left| (\rho_1 - \rho_\circ) \int_{V_1} e^{-i\mathbf{q}\cdot\mathbf{r}}\ d\mathbf{r} + (\rho_1 - \rho_\circ) \int_{V_2} e^{-i\mathbf{q}\cdot\mathbf{r}}\ d\mathbf{r} \right|^2 \right\rangle$$

Giving

$$I(\mathbf{q}) = (\rho_1 - \rho_\circ)^2\ [F_1^2(\mathbf{q}) + F_2^2(\mathbf{q}) + F_1(\mathbf{q})F_2(\mathbf{q})\ \frac{\sin(\mathbf{q}\cdot\mathbf{r_{12}})}{\mathbf{q}\cdot\mathbf{r_{12}}}]$$

Compound particles:

Modelled as an assembly of uniform subunits



examples:
nucleosomes, protein/DNA complexes
ribosomes: protein/RNA complexes

$$I(\mathbf{q}) = \int_V \int_V \langle \delta\rho(\mathbf{r})\, \delta\rho(\mathbf{r}')\rangle e^{-i\mathbf{q}\cdot\mathbf{r}}\, d\mathbf{r}d\mathbf{r}'$$
$$= \left\langle \left| \int_V \delta\rho(\mathbf{r})\, e^{-i\mathbf{q}\cdot\mathbf{r}}\, d\mathbf{r}d\mathbf{r}' \right|^2 \right\rangle$$

With $V = V_1 + V_2$

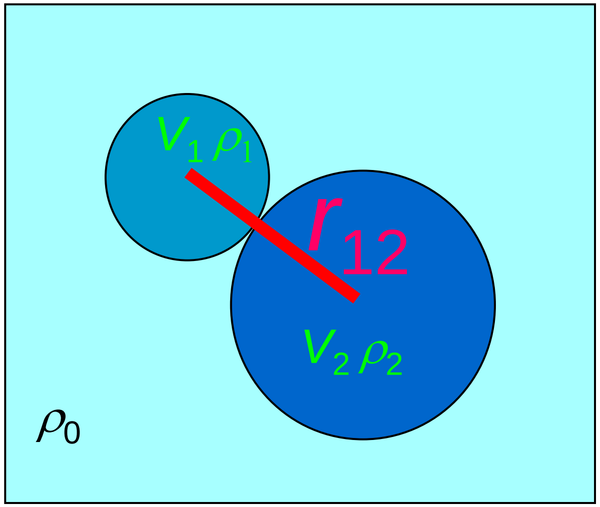
Monte Carlo type of data-analysis

$$I(\mathbf{q}) = \left\langle \left| (\rho_1 - \rho_\circ) \int_{V_1} e^{-i\mathbf{q}\cdot\mathbf{r}}\, d\mathbf{r} + (\rho_1 - \rho_\circ) \int_{V_2} e^{-i\mathbf{q}\cdot\mathbf{r}}\, d\mathbf{r} \right|^2 \right\rangle$$

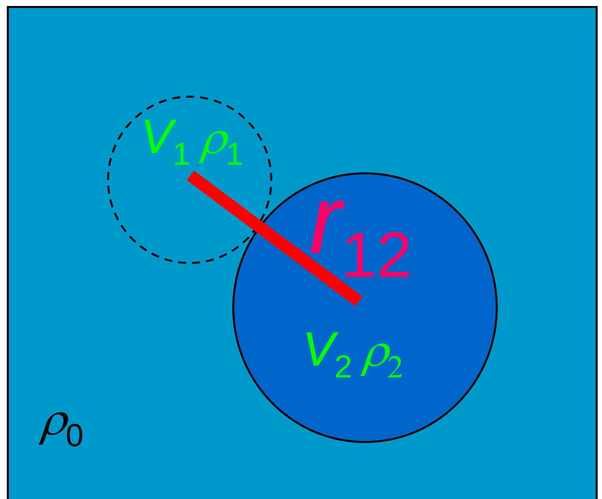
Giving

$$I(\mathbf{q}) = (\rho_1 - \rho_\circ)^2 \left[F_1^2(\mathbf{q}) + F_2^2(\mathbf{q}) + F_1(\mathbf{q})F_2(\mathbf{q}) \frac{\sin(\mathbf{q}\cdot\mathbf{r_{12}})}{\mathbf{q}\cdot\mathbf{r_{12}}}\right]$$

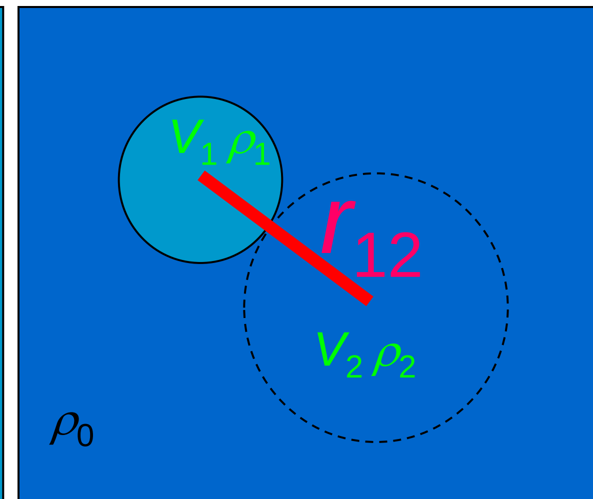
Compound Particle
Using contrast variation



$$
\begin{aligned}
I(\mathbf{q}) &= (\rho_1-\rho_\circ)^2 F_1^2(\mathbf{q}) + (\rho_2-\rho_\circ)^2 F_2^2(\mathbf{q}) + \\
& (\rho_1-\rho_\circ)(\rho_2-\rho_\circ)\ F_1(\mathbf{q})F_2(\mathbf{q})\ \frac{\sin(\mathbf{q}\cdot\mathbf{r_{12}})}{\mathbf{q}\cdot\mathbf{r_{12}}}
\end{aligned}
$$



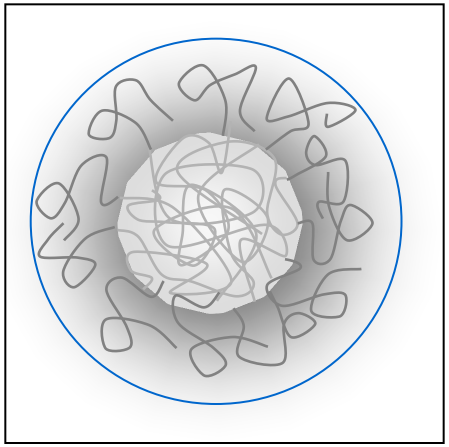
$$I(\mathbf{q}) = (\rho_1-\rho_\circ)^2 F_1^2(\mathbf{q})$$



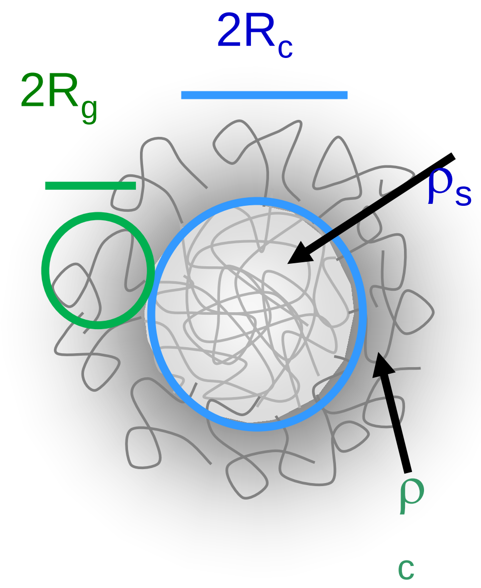
$$I(\mathbf{q}) = (\rho_2-\rho_\circ)^2 F_2^2(\mathbf{q})$$

Measurements in the three conditions gives
the structure of the individual subunits,
and the distance r_{12}

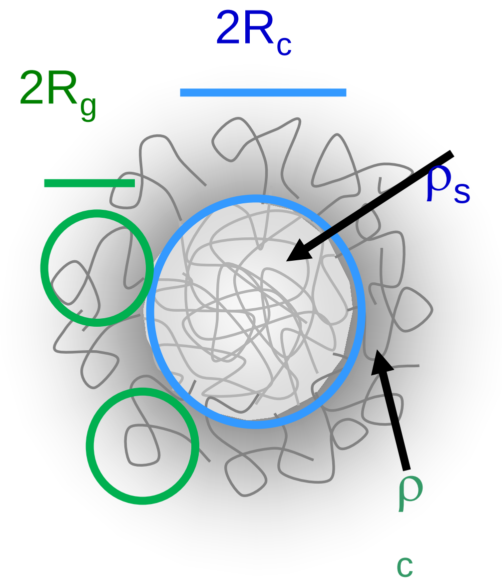
Form factor of Micelle modeled as Sphere + Corona with Coils

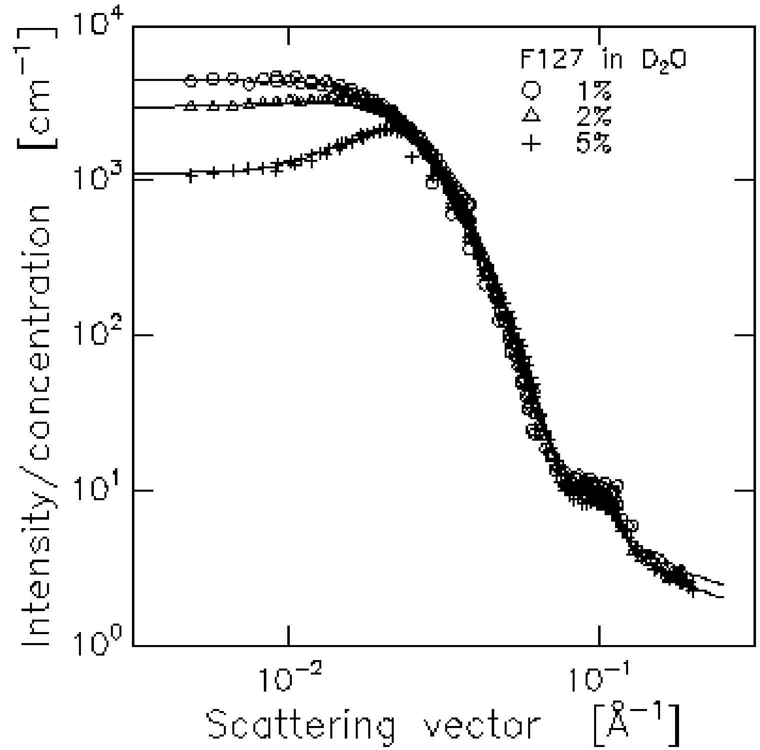


COMPOUND PARTICLE
build up
spheres + coils



Compound particle:
Form factor of Micelle





$F_{mic}(q) = n^2\rho_s^2F_s(q) + n\rho_c 2F_c(q) + n(n-1)\,\rho_c^2S_{cc}(q) + 2n\rho_s\rho_c S_{sc}(q)$

with

$F_c(q) = x^{-2}(e^{-x}+x-1),\ \ x=(qR_g)^2$ Gaussian chain

$F_s(q) = [3(qR_c)^3\{\sin(qR_c)-qR_c\cos(qR_c)\}]^2 = \Phi_s^2$ Solid Sphere

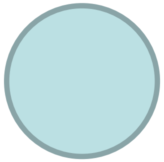
$S_{cc}(q) = \Phi_s\, x^{-1}(1-e^{-x})\sin(qR) / qR$

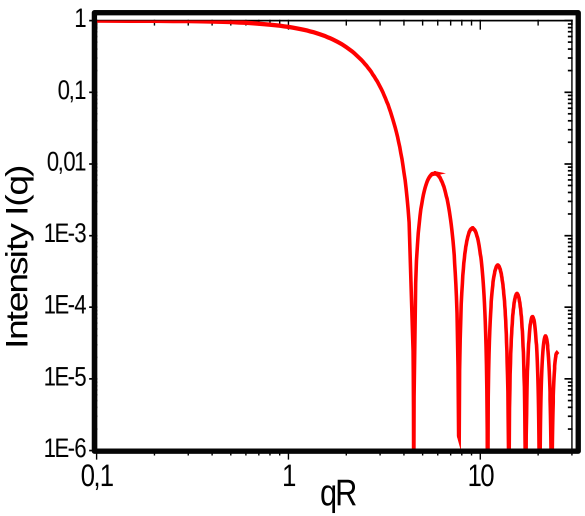
$S_{sc}(q) = x^{-2}(1-e^{-x})\,[\sin(qR) / qR]^2$

Form Factor
of
Simple Objects

Cylinder

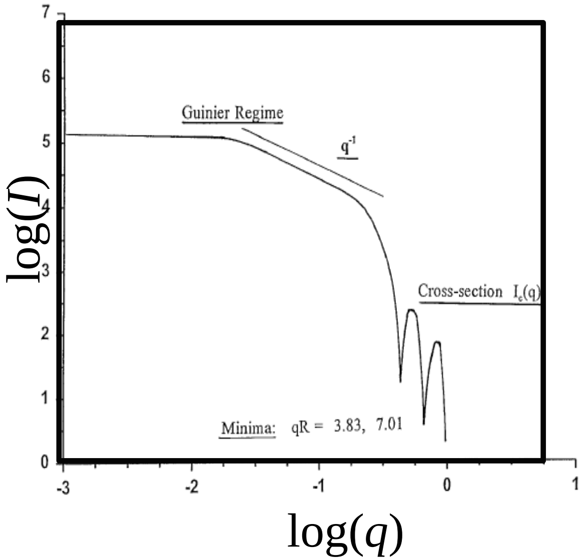
Sphere





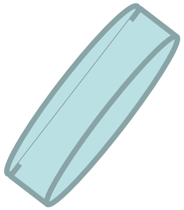
$$qR_{min,1} = 4.49$$

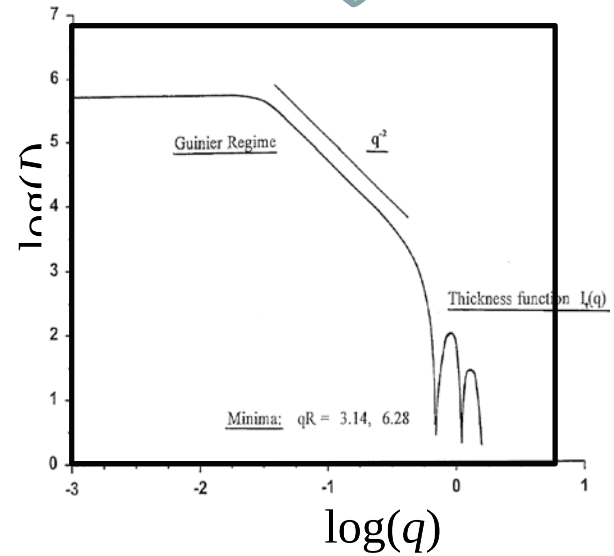
Rod



$$qR_{min,1} = 3.38$$

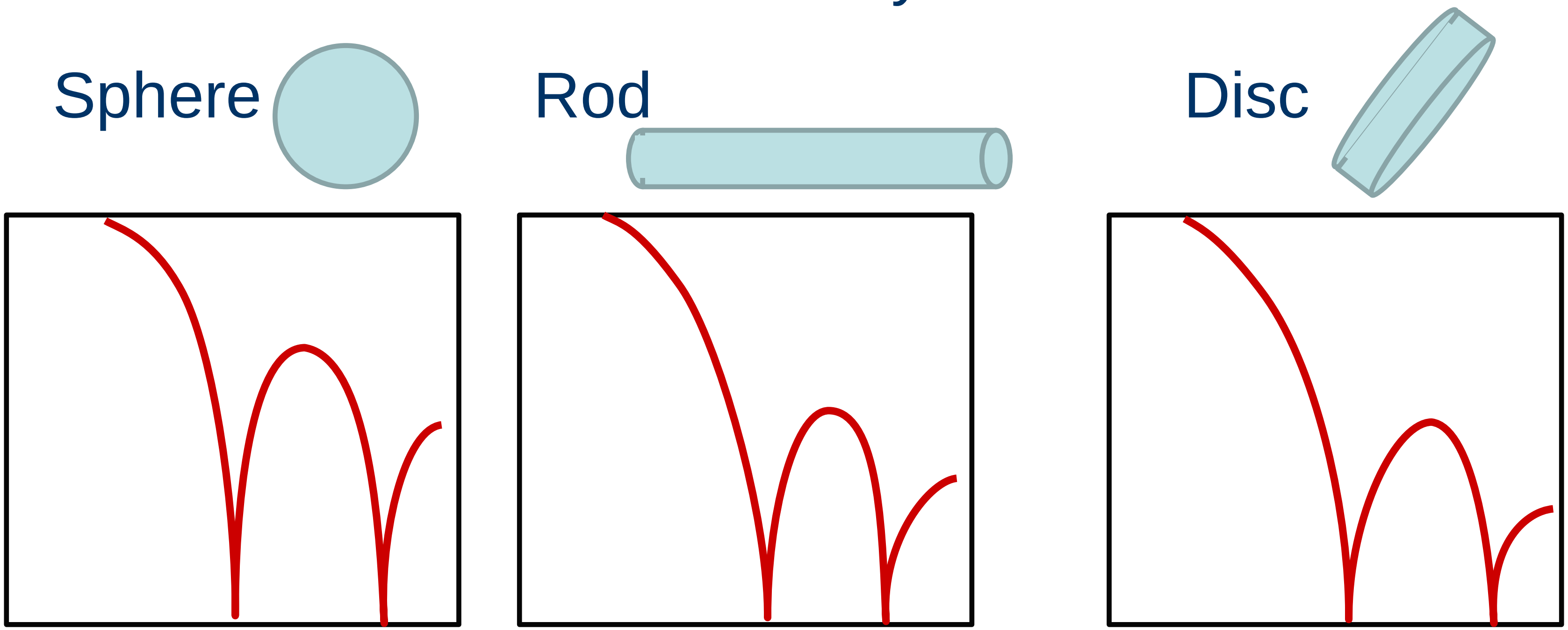
Disc





$$qR_{min,1} = 3.14$$

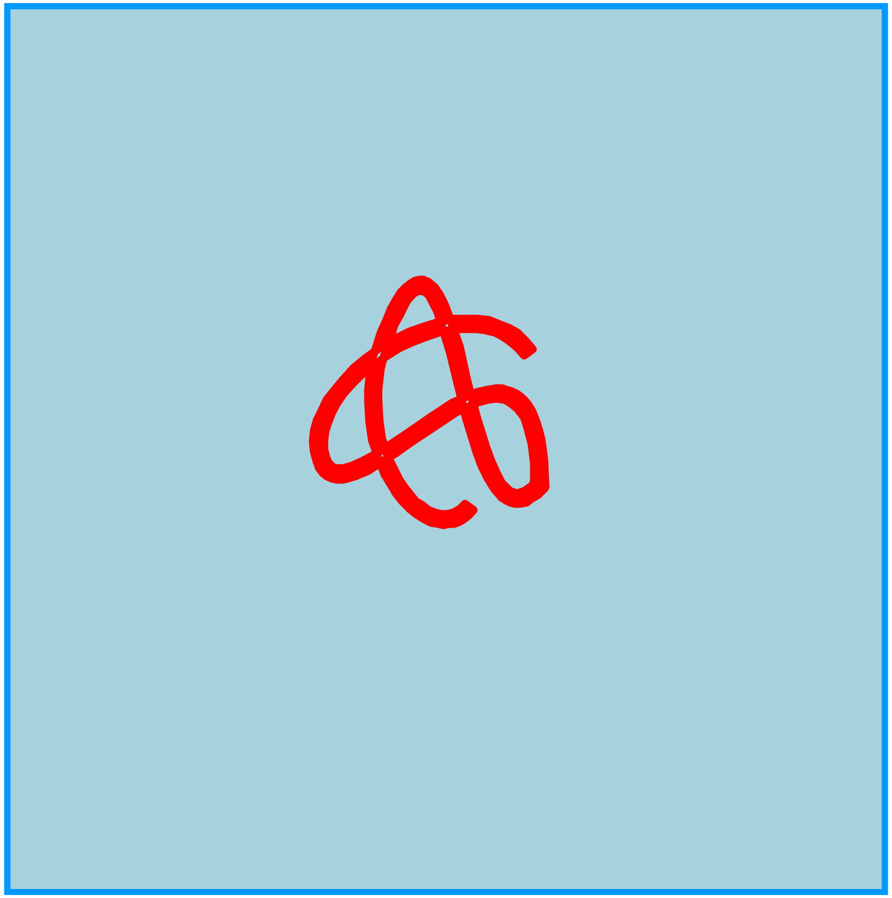
Cylinder

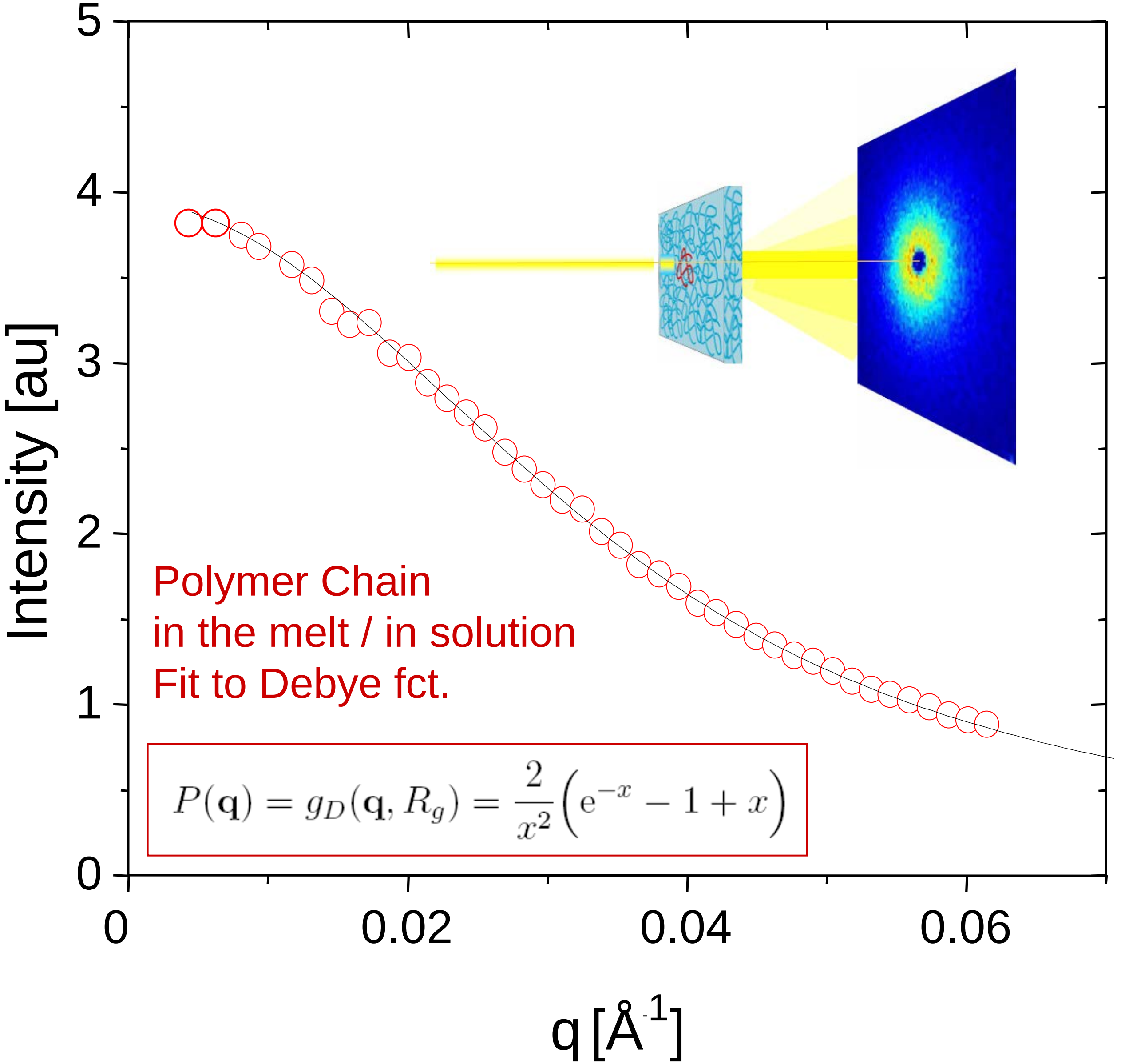


Sphere	Rod	Disc
$qR_{min,1} = 4.49$	$qR_{min,1} = 3.38$	$qR_{min,1} = 3.14$
$qR_{min,2}/qR_{min,1} = 1.72$	$qR_{min,2}/qR_{min,1} = 1.83$	$qR_{min,2}/qR_{min,1} = 2.00$
qR_{min2}-qR_{min1}=3.20	qR_{min2}-qR_{min1}=3.18	qR_{min2}-qR_{min1}=3.14

Form factor of Polymer Chain

in solution





Intensity [au]
0
1
2
3
4
5
0
0.02
0.04
0.06
q [Å-1]
Polymer Chain
in the melt / in solution
Fit to Debye fct.
$P(\mathbf{q}) = g_D(\mathbf{q}, R_g) = \frac{2}{x^2}\left(e^{-x} - 1 + x\right)$

Low-q approximation for a polymer coil

Form factor for Gaussian polymer coil

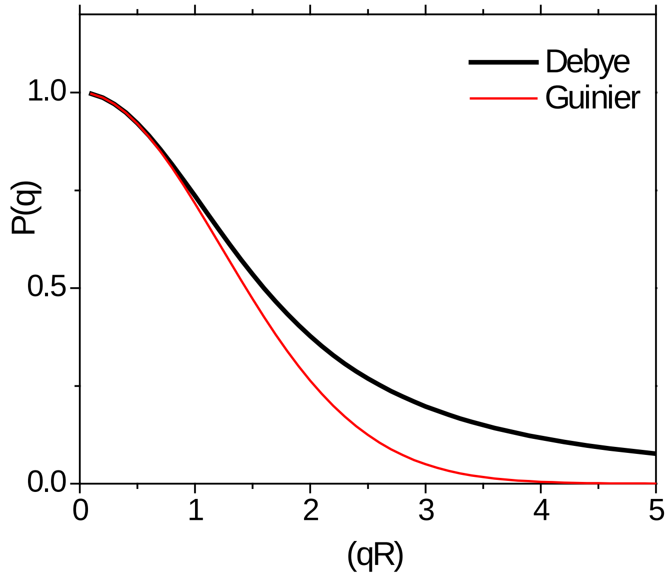
$$P(q) = \frac{2}{x^2}\left[e^{-x} - 1 + x\right] \qquad \text{with } x = q^2 R_g^2.$$

in the low-q regime $x << 1$:

$$\begin{aligned} P(q) &= \frac{2}{x^2}\left[e^{-x} - 1 + x\right] \\ &\approx \frac{2}{x^2}\left[1 - x + \frac{1}{2}x^2 - \frac{1}{6}x^3 + \ldots - 1 + x\right] \\ &\approx 1 - \frac{1}{3}x \\ &= 1 - \frac{1}{3}q^2 R_g^2 \end{aligned}$$

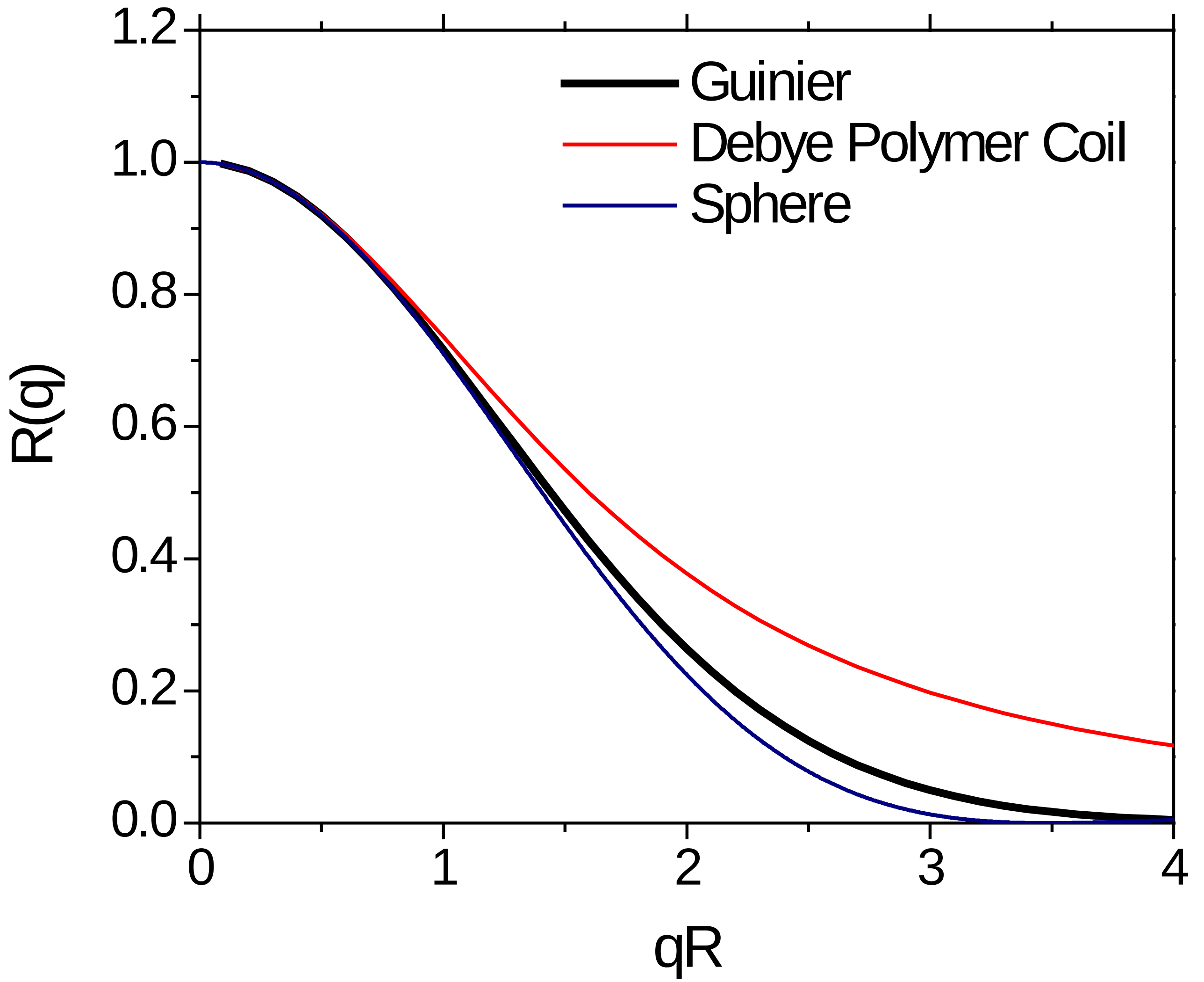
which may be rewritten in exponential approximation:

$$\boxed{P(q) \approx \exp[-\frac{1}{3}q^2 R_g^2]}$$



i.e. in the usual Guinier form

Guinier Approximation



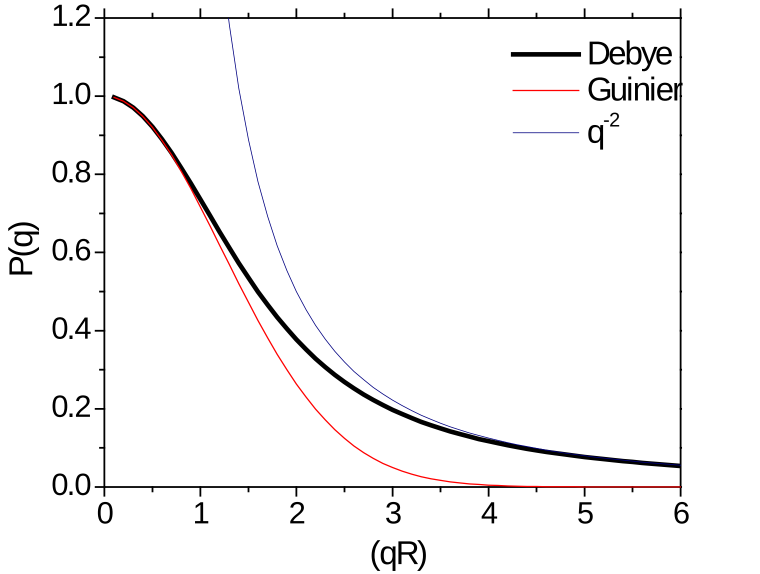
High-q approximation for a polymer coil

Form factor for Gaussian polymer coil

$$\boxed{P(q) = \frac{2}{x^2}\left[e^{-x} - 1 + x\right]} \quad \text{with } x = q^2 R_g^2.$$

in the low q-regime, $x \ll 1$ ($x<1$):

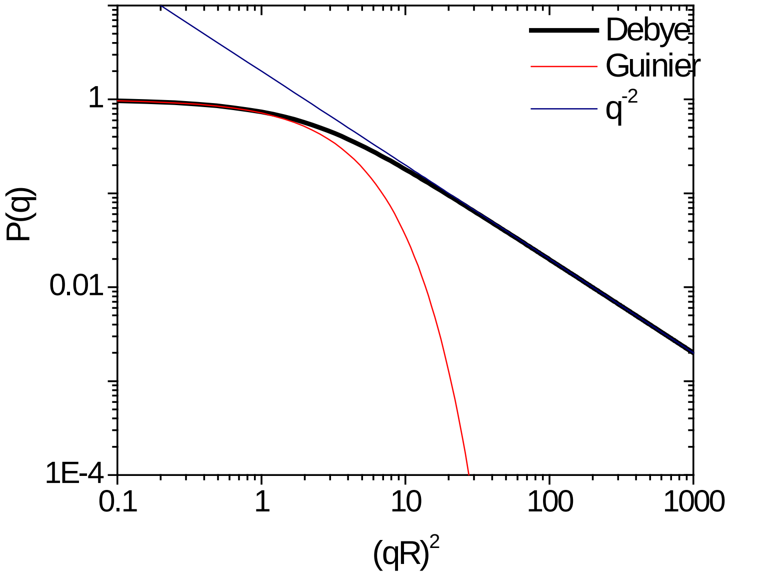
$$\boxed{P(q) \approx \exp[-\frac{1}{3} q^2 R_g^2]}$$



in the high q-regime, x>>1 (x>10):

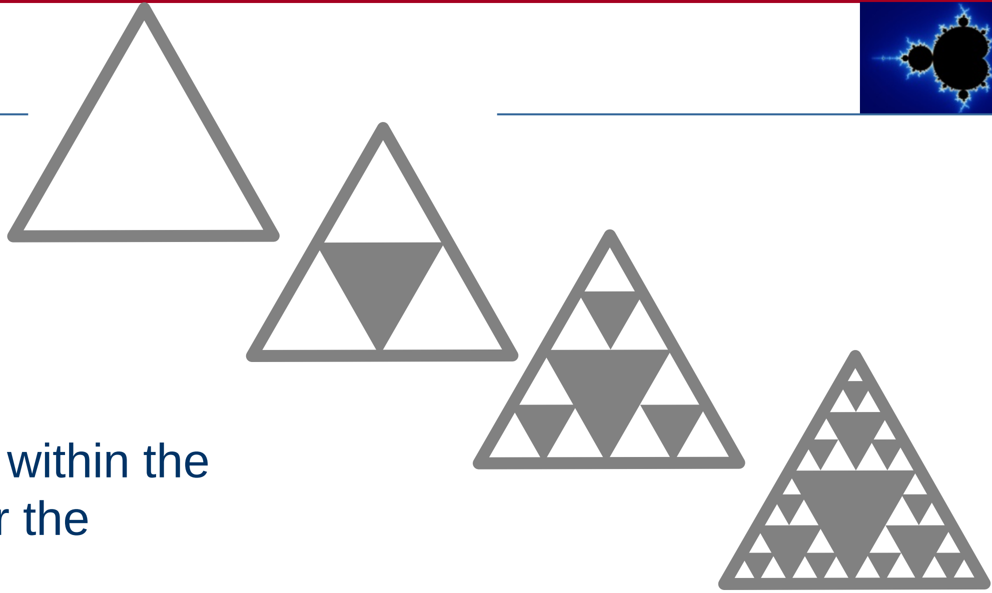
$$P(q) \approx \frac{2}{x^2}[0 - 1 + x] = \frac{2}{x}$$

$$\boxed{P(q) = 2R_g^{-2} q^{-2}}$$



i.e. fractal with fractal dimension 2.

Form factor of Mass Fractal



The mass scale with radius as:

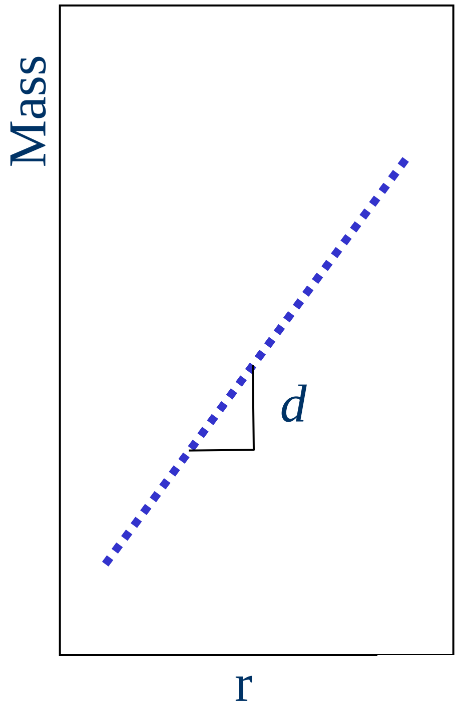
$$M \propto r^d$$

Assume that system obey the fractal law within the 3D Euclidian volume, give the formula for the correlation function:

$$\gamma(r)$$

Calculate thereby the Scattering Function using the formula:

$$I(q) \;=\; \int \gamma(r) \frac{\sin(qr)}{qr}\, r^2 \, dr$$



Form factor of Mass Fractal

The mass (scattering power) scale with radius as:

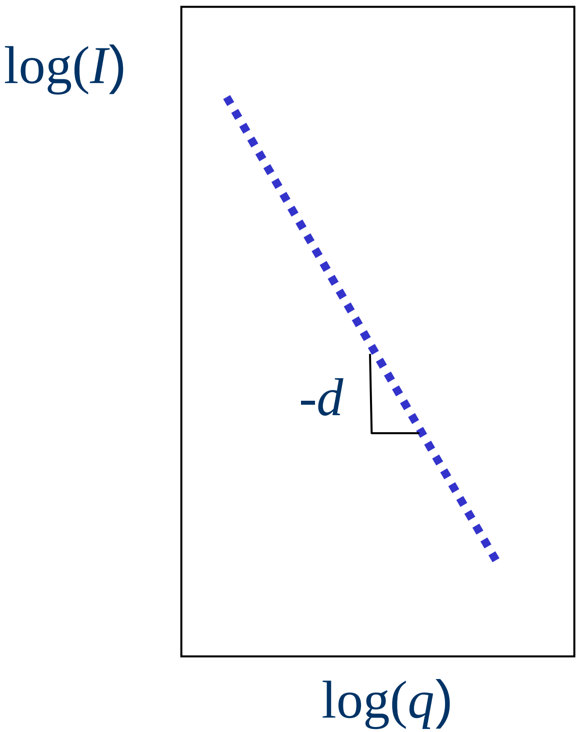
$$M \propto r^d$$

and thereby the correlation function

$$\gamma(r) \propto M/V \propto r^{d-3}$$

which inset into the equation for scattering gives

$$\begin{aligned} I(q) &= \int \gamma(r) \frac{\sin(qr)}{qr} r^2\, dr \\ &\sim \int (qr)^{d-3+2} \frac{sin(qr)}{qr} d(qr) \cdot q^{-d+3-2-1} \\ &= cst \cdot q^{-d} \end{aligned}$$



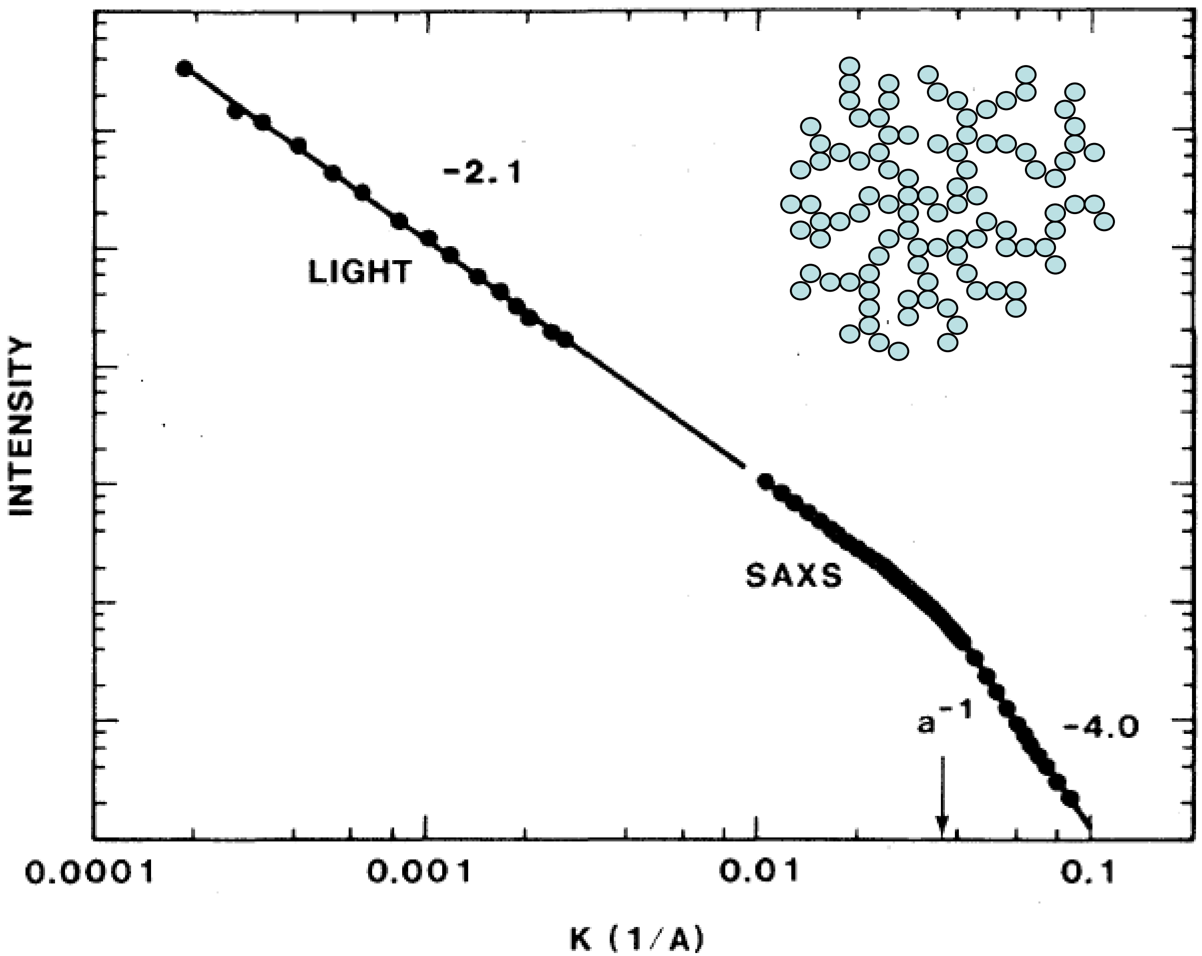
Form factor of Mass Fractal

Colloidal aggregates
diffusion limited aggregation

PHYSICAL REVIEW LETTERS

Fractal Geometry of Colloidal Aggregates

Dale W. Schaefer and James E. Martin
Pierre Wiltzius and David S. Cannell



PRL 52, 2371 (1984)

Fractals

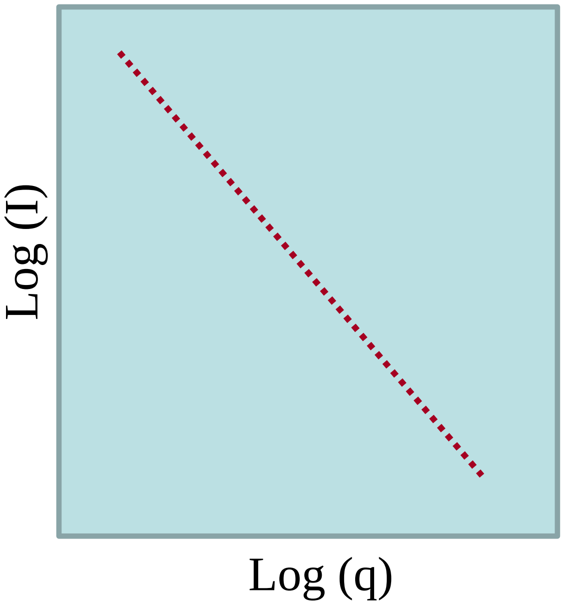
$$\boxed{I(q) \sim q^{-d}}$$

Mass-fractal **1<d<3**

$$I(q) \sim q^{-d} = q^{-dm}$$

Surface Fractal **3<d<4**

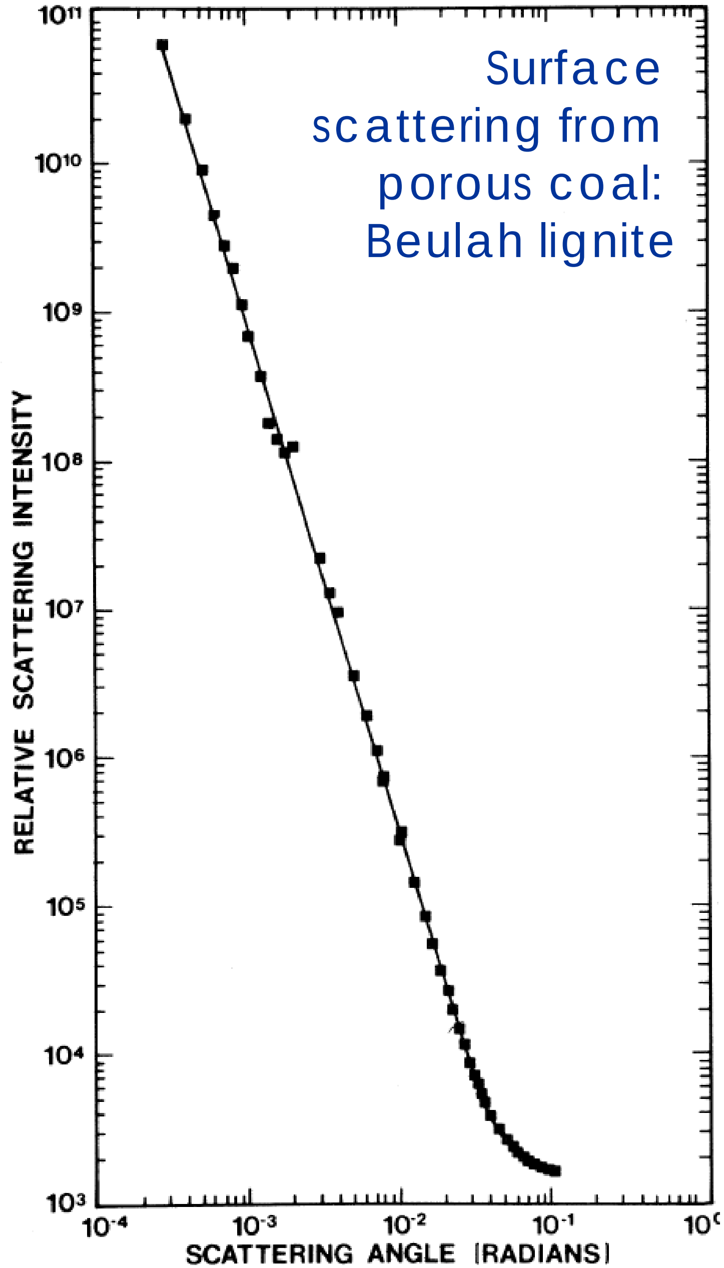
$$I(q) \sim q^{-d} = q^{-(6-d_S)}$$



with surface fractal dimension d_s

$$2 \leq d_s < 3$$

Surface Fractal



VOLUME 53, NUMBER 6 PHYSICAL REVIEW LETTERS 6 AUGUST 1984

Small-Angle X-Ray-Scattering Investigation of Submicroscopic Porosity with Fractal Properties

Harold D. Bale[a] and Paul W. Schmidt

Bale and Schmidt showed that the Porod law can be generalized to non-smooth surfaces, to the form

$$I(q) \propto q^{-(6-d_s)}$$

with the surface fractal:

$$2 \leq d_s < 3$$

Linear in log-log plot:

$$I(q) \sim q^{-3.44}$$

corresponding to a surface fractal dimension:

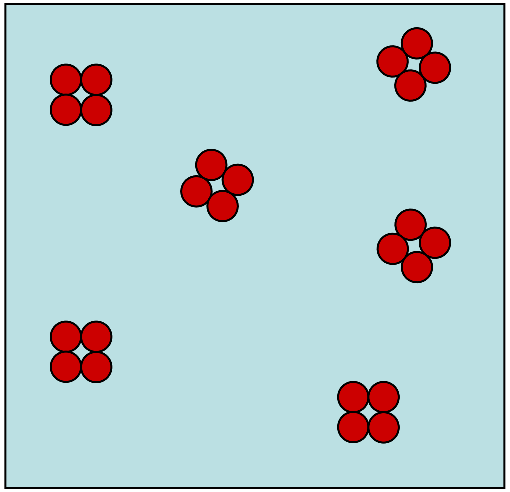
$$d_s = 6 - 3.44 = 2.56$$

PRL 53, 596 (1984)

Structure Factor

Decomposition into intra and inter correlations

$$I(\mathbf{q}) = \sum_{i=1}^{M}\sum_{j=1}^{M}\sum_{p=1}^{n}\sum_{q=1}^{n}\left\langle (\Delta\rho)^2 \; \exp[-i\mathbf{q}\cdot(\mathbf{r}_{p,i} - \mathbf{r}_{q,j})]\right\rangle$$



assume spherical symmetry,
dilute mono-disperse ensemble

$$I(\mathbf{q}) \;=\; (\Delta\rho)^2\, nM^2 \cdot \underbrace{\frac{1}{M^2}\sum_{i,j}\left\langle \exp[-i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)]\right\rangle}\; \underbrace{\left[1 \,+\, \frac{1}{n}\sum_{p\neq q}\left\langle \exp[-i\mathbf{q}\cdot(\mathbf{r}_p - \mathbf{r}_q)]\right\rangle\right]}$$

intra particle correlations
giving information on
particle shape

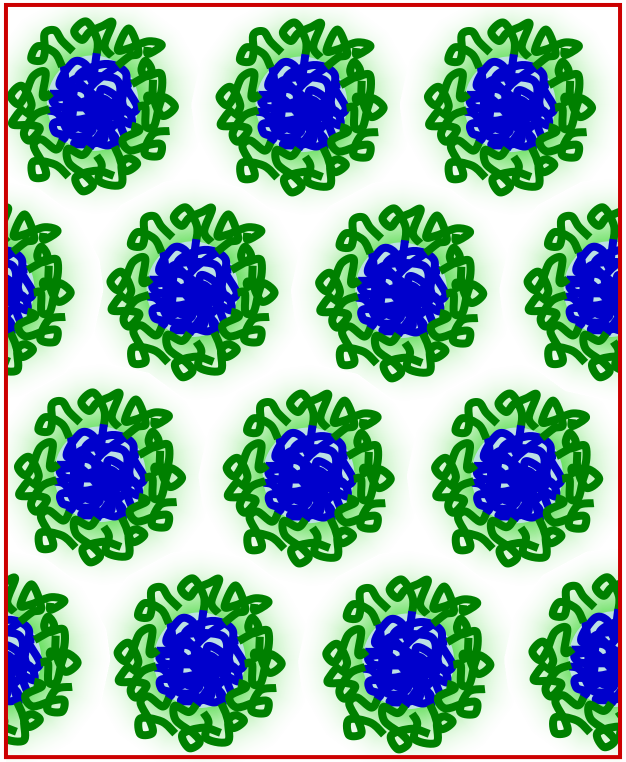
inter particle correlations
approach 1 for dilute systems

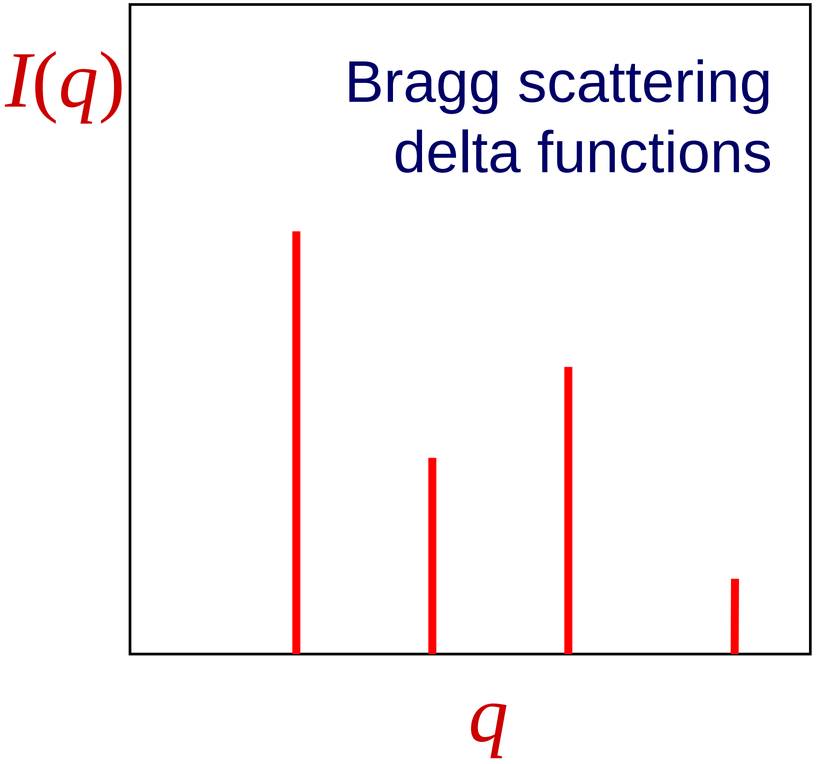
$$I(\mathbf{q}) = \underbrace{\boxed{(\Delta\rho)^2\, nM^2}}_{\text{pre factor}}\;\underbrace{\boxed{P(\mathbf{q})}}_{\text{form factor}}\;\underbrace{\boxed{S(\mathbf{q})}}_{\text{structure factor}}$$

Structure factor

$$I(\mathbf{q}) = (\Delta\rho)^2\, nM^2\, P(\mathbf{q})S(\mathbf{q})$$

Ordered, crystalline structure

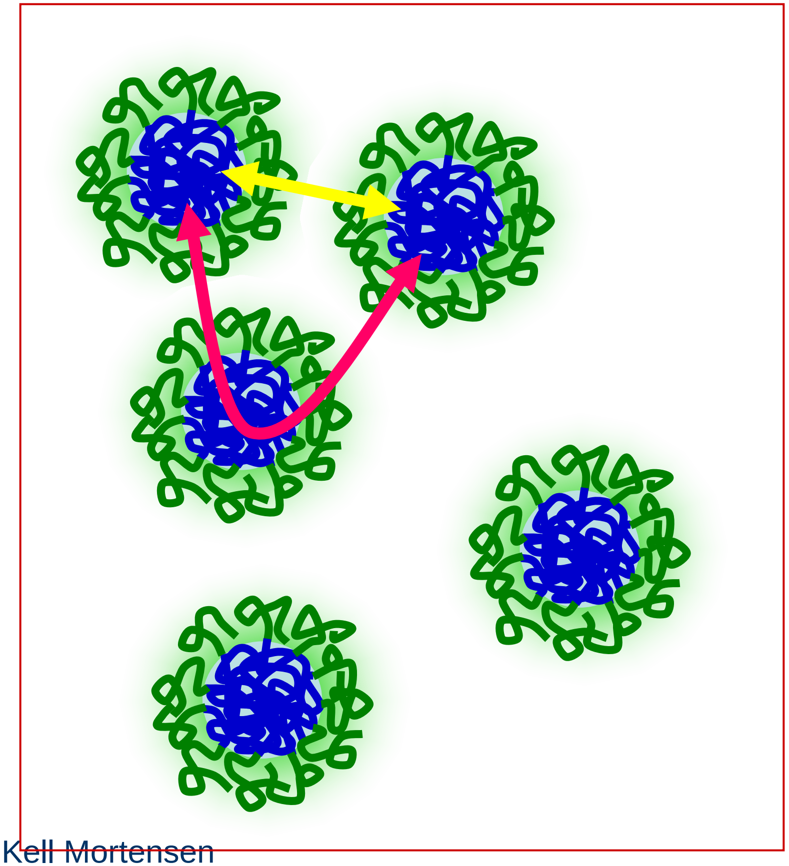


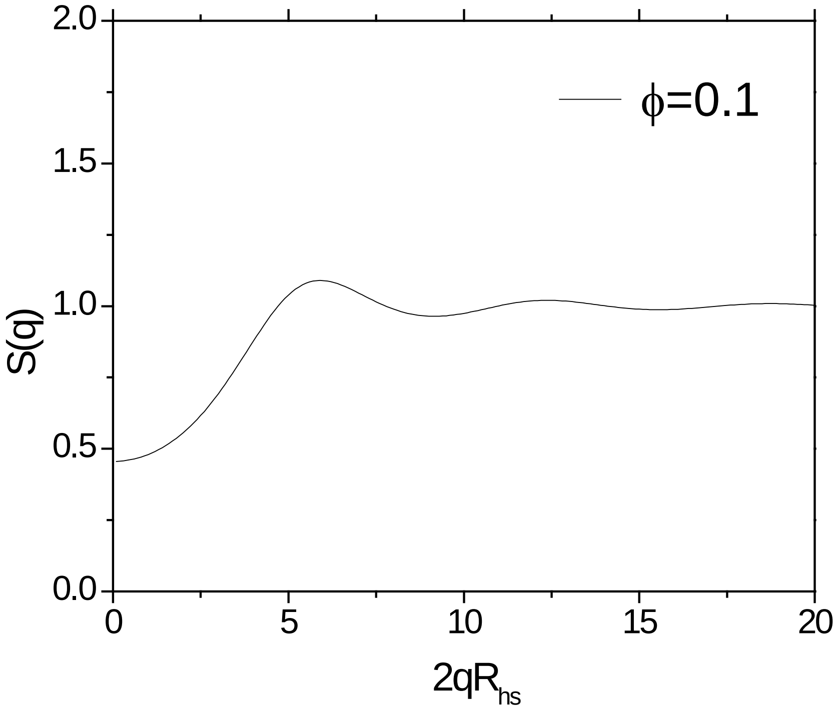


Structure factor

$$I(\mathbf{q}) = (\Delta\rho)^2 \, nM^2 \; P(\mathbf{q}) S(\mathbf{q})$$

$$S(\mathbf{q}) = \left[1 \; + \; \sum_{p \neq q} \left\langle \exp[-i\mathbf{q} \cdot (\mathbf{r}_p - \mathbf{r}_q)] \right\rangle \; \right]$$

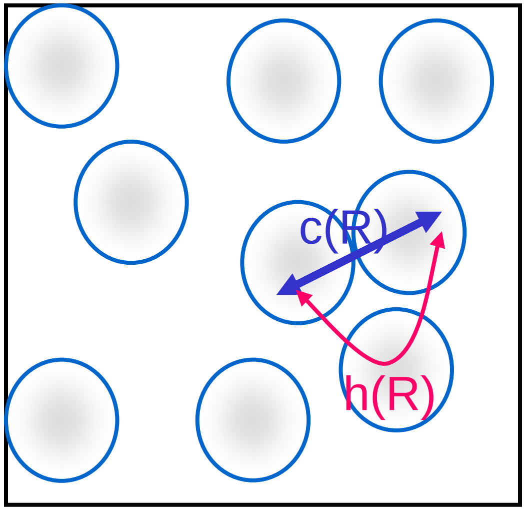




Structure factor

$S(q) = 1 + 4\pi N \int h(R) \sin(qR)/qR \, R^2 \, dR$

h(R) correlation function



Ornstein Zernike Approximation

$h(R_{12}) = c(R_{12}) + n \int c(R_{13}) \, h(R_{23}) \, dR_3$

c(R) direct short range correlation

Percus Yevick Approximation

$c(R) = [e^{-\Phi/kT)}-1] \, e^{\Phi/kT} \, [h(R)+1], \quad \Phi = \Phi(R)$

Hard-sphere interaction

$c(R) = [\alpha + \beta \, (R/R_{hs}) + \gamma \, (R/R_{hs})^2])$, α,β,γ function of volume fraction ϕ

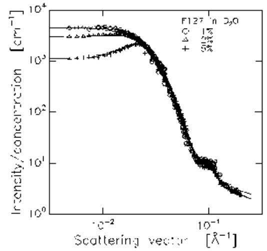
$S(q) = [1 + 24 \, \phi \, G(2qR_{hs})/2qR_{hs}]^{-1}$

Thus, Intensity $I(q) = P(q) \, S(q)$

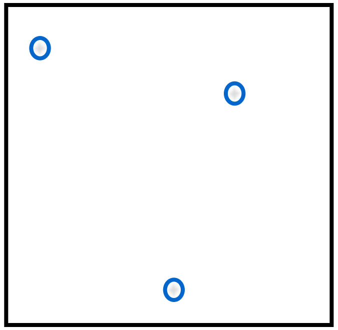
only depending on core size R_c, Volume fraction ϕ and Interaction distance R_{hs}

Structure factor

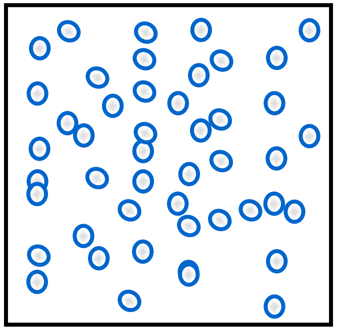
Hard-sphere Perkus-Yevick

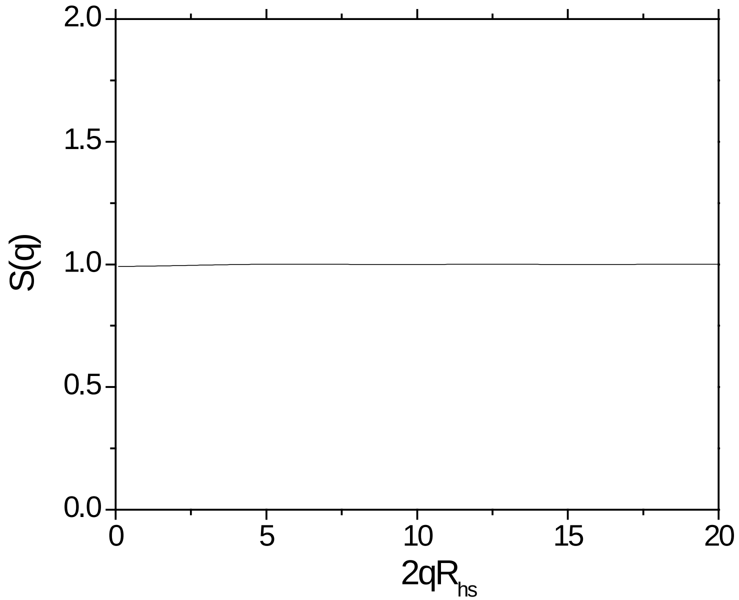


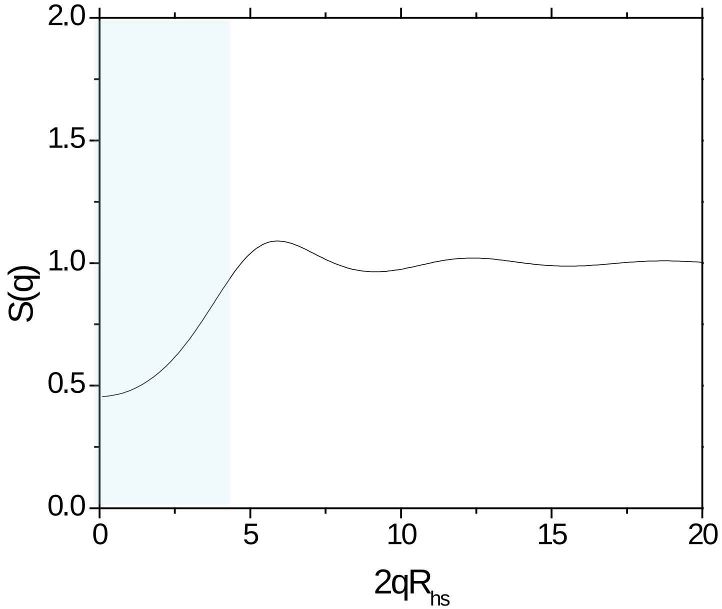
Volume fraction 0.1%



Volume fraction 10%



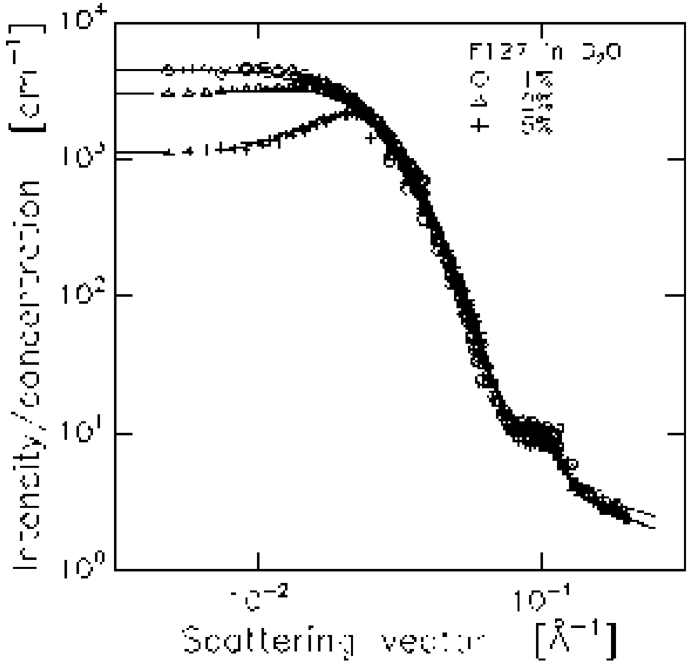


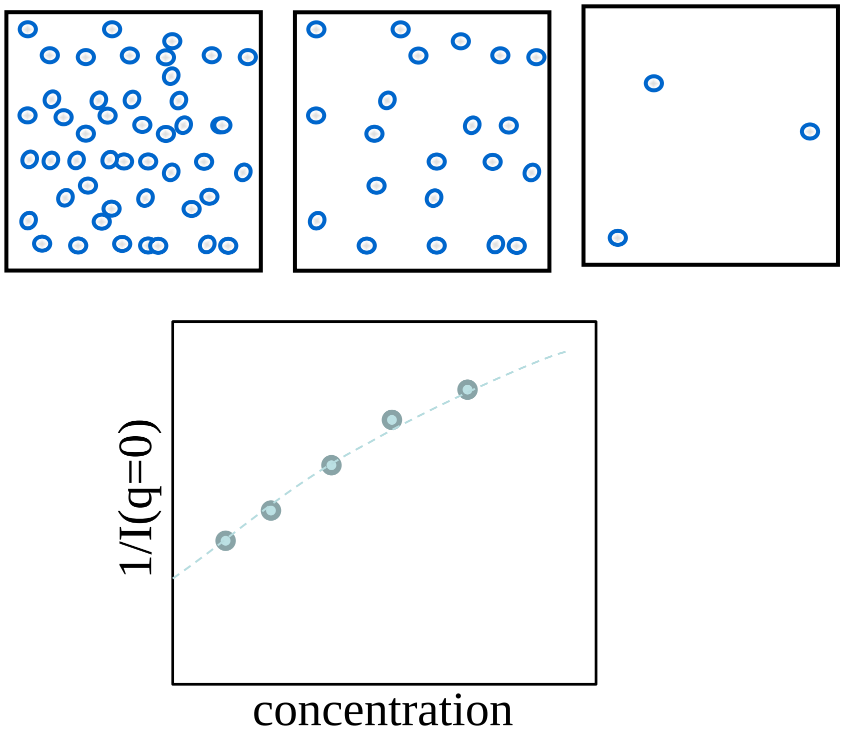


Correlation Hole

Structure factor

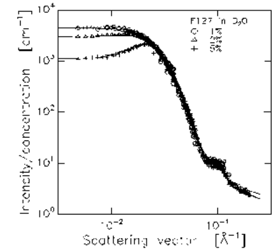
Measure a concentration series to get the correct form factor and zero-q instensity (Molar mass)

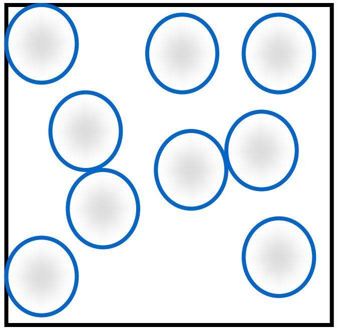


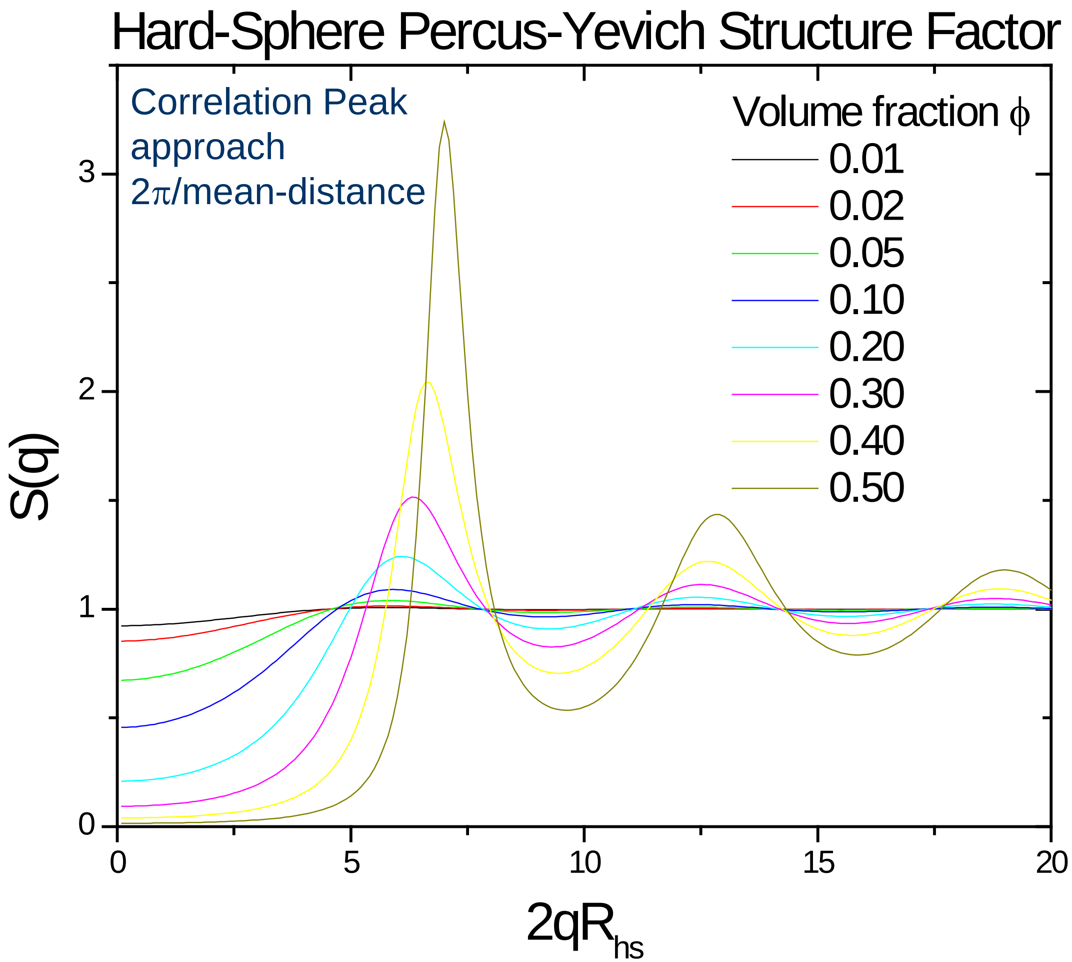


Structure factor

Hard-sphere Perkus-Yevick

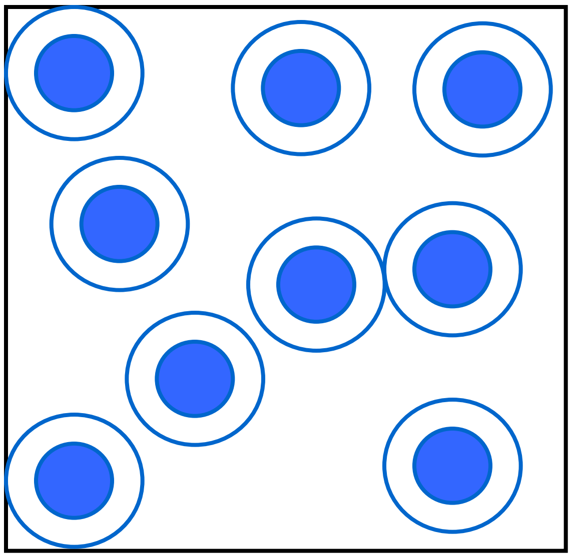




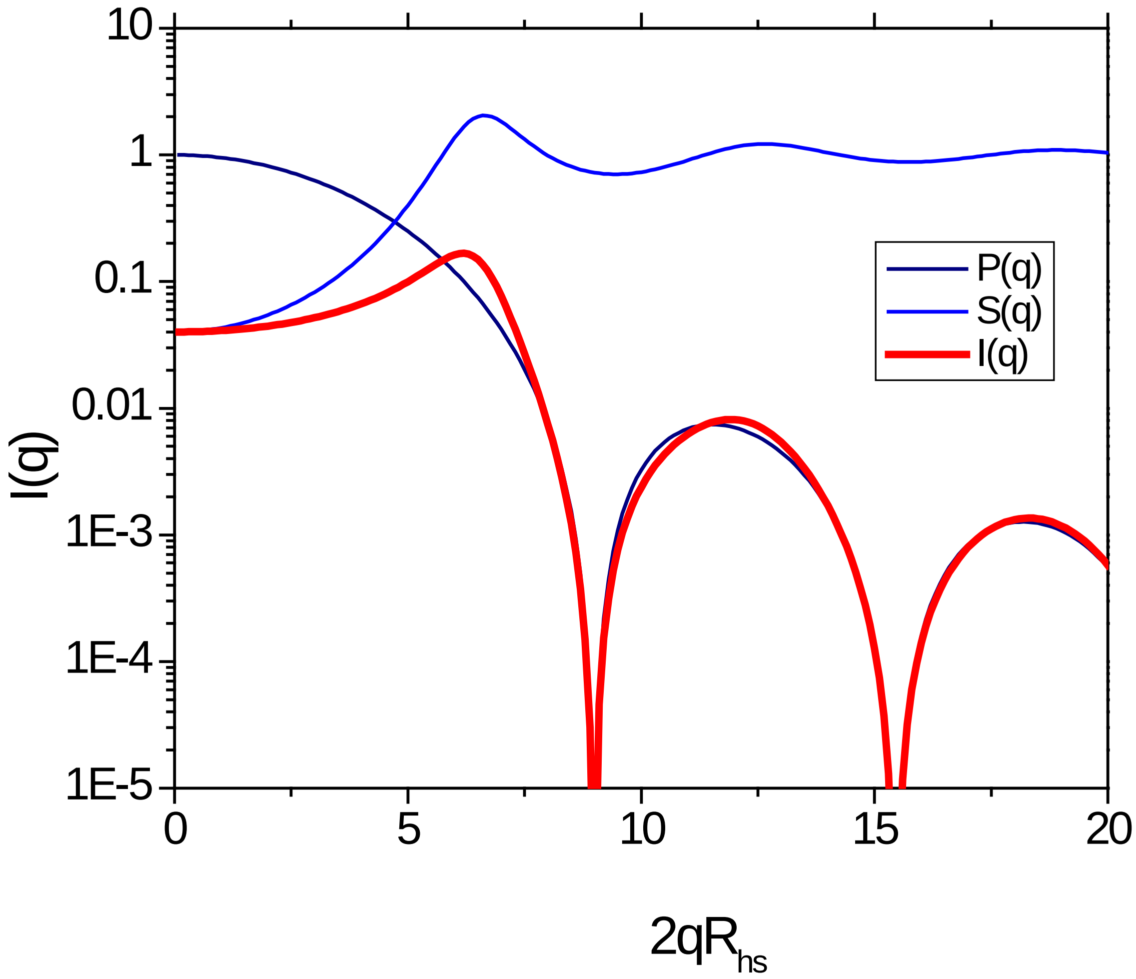


Scattering Function Hard-sphere Perkus-Yevick

$$I(\mathbf{q}) = \mathrm{b}^2 \; P(\mathbf{q})S(\mathbf{q})$$



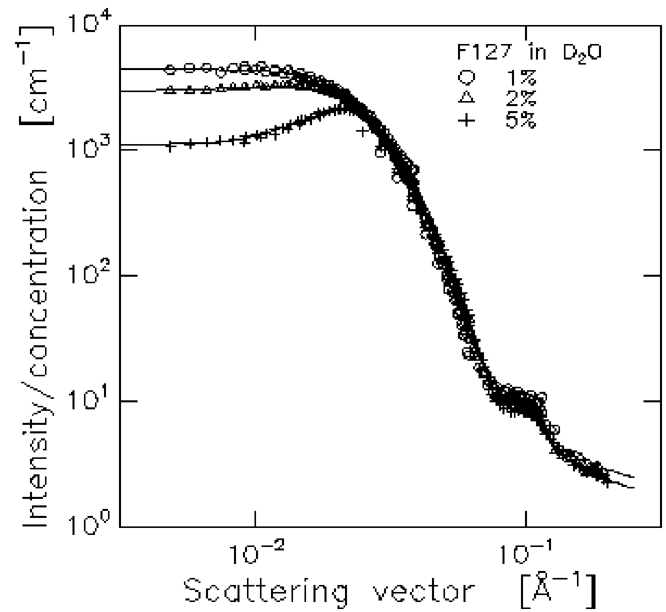
$R_{hs} = 2R_c$
$\phi=0.4$

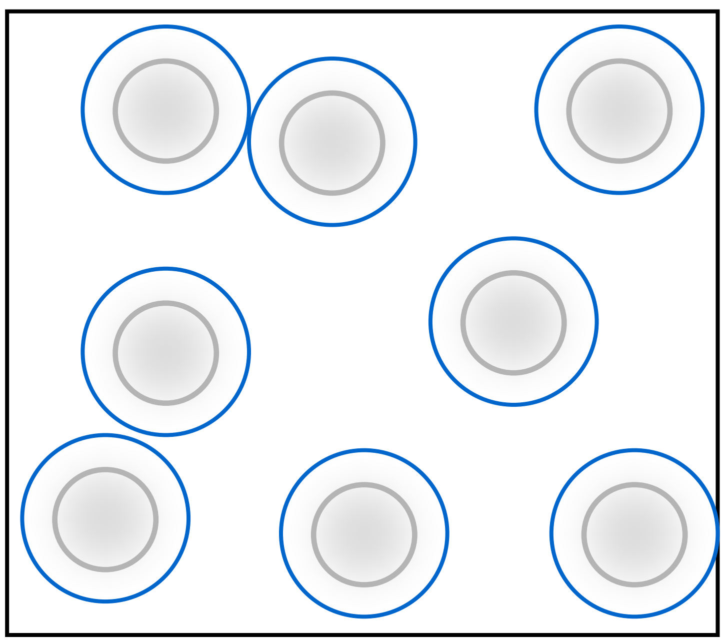


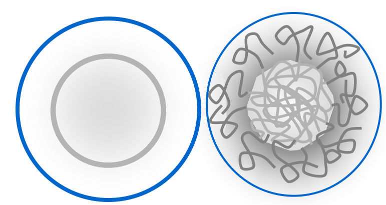
Structure Factor:

$$I(q) = nM^2 \Delta\rho^2 P(q) S(q)$$

$$I(q) = nM^2 \Delta\rho^2 P(q,Rc) S(q,Rhs, \phi)$$



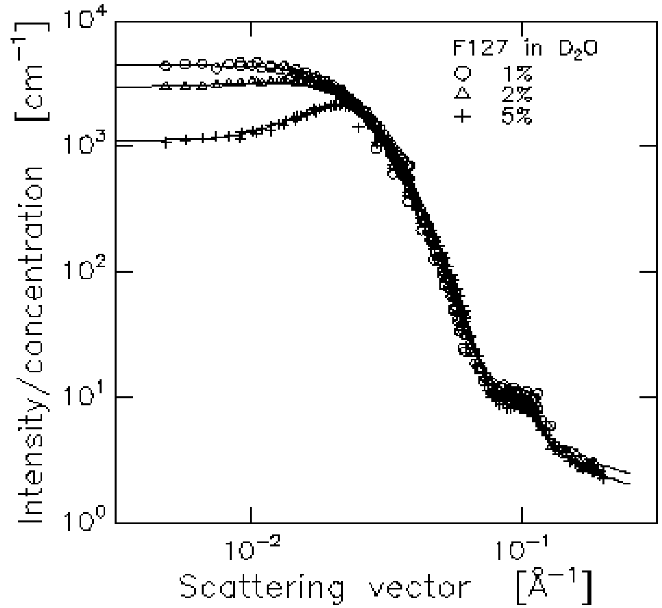




Structure factor

$S(q) = 1 + 4\pi N \int h(R) \sin(qR)/qR\ R^2\, dR$

$h(R)$ correlation function



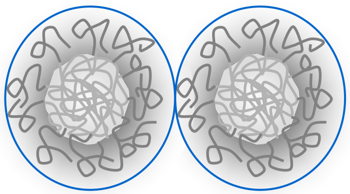
Ornstein Zernike Approximation

$h(R_{12}) = c(R_{12}) + n \int c(R_{13})\, h(R_{23})\, dR_3$

$c(R)$ direct short range correlation

Percus Yevick Approximation

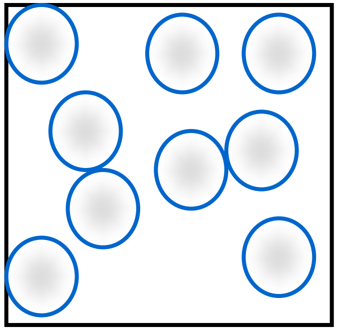
$c(R) = [e^{-\Phi/kT)}-1]\, e^{\Phi/kT}\, [h(R)+1], \quad \Phi = \Phi(R)$



Hard-sphere interaction

$c(R) = [\alpha + \beta\, (R/R_{hs}) + \gamma\, (R/R_{hs})^2]),$

α,β,γ function of volume fraction ϕ



$S(q) = [1 + 24\, \phi\, G(2qR_{hs})/2qR_{hs}]^{-1}$

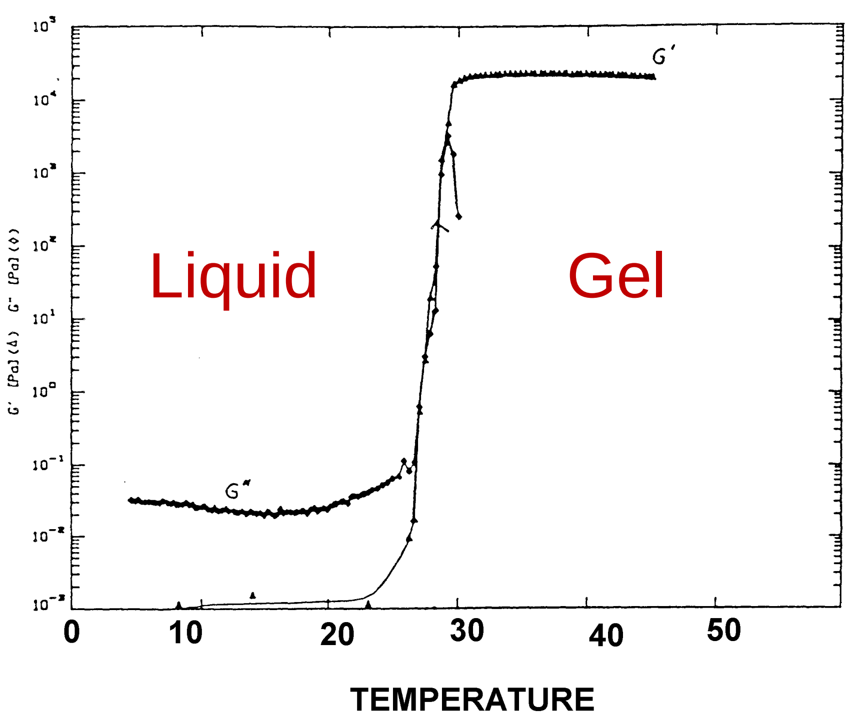
Thus, Intensity $I(q) = P(q)\, S(q)$

only depending on core size R_c,

Volume fraction ϕ and Interaction distance R_{hs}

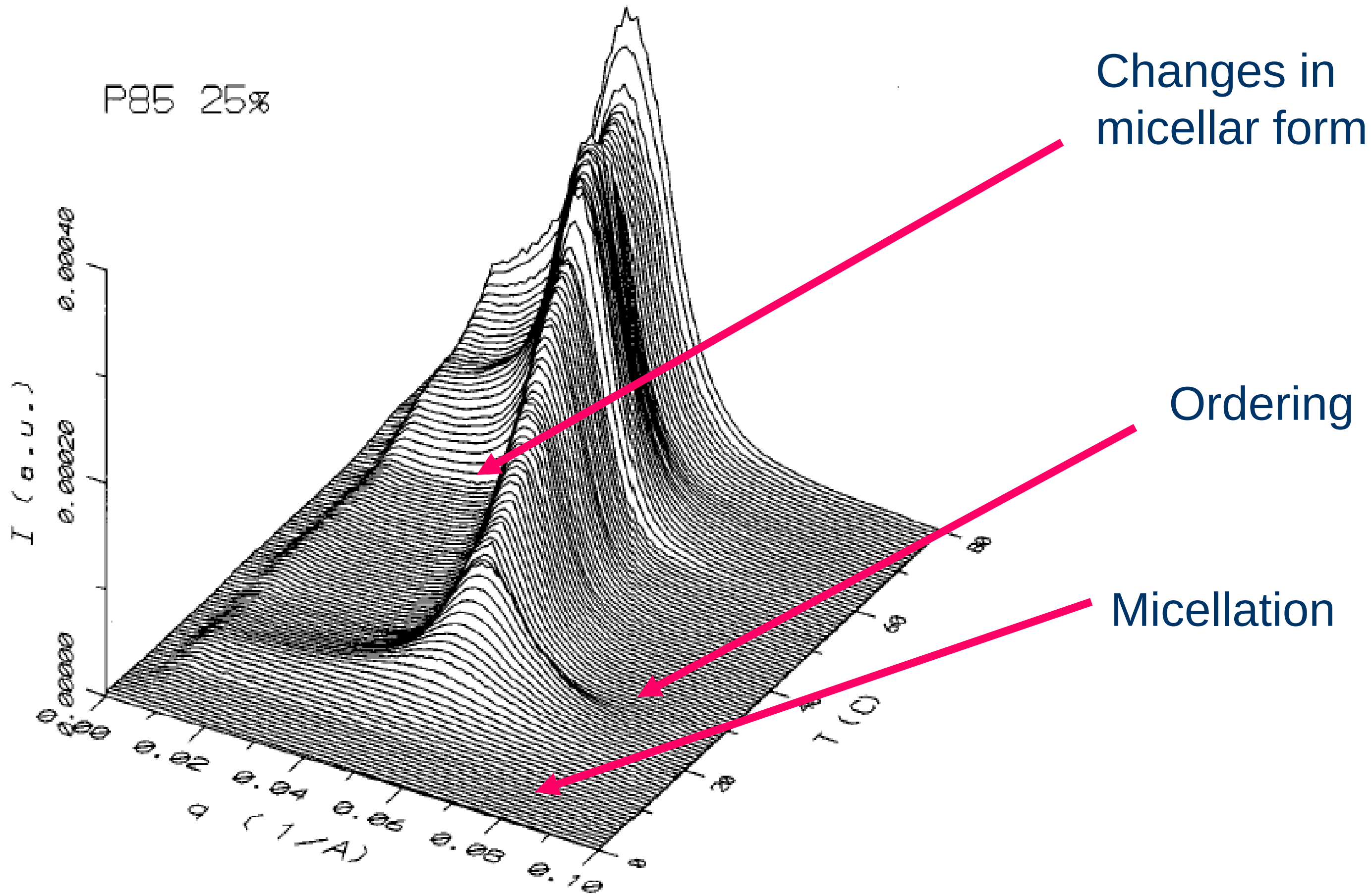
Measured Scattering Function as a function of temperature

PEO-PPO-PEO (P85) 25 % in D_2O



Measured Scattering Function as a function of temperature

PEO-PPO-PEO (P85) 25 % in D_2O



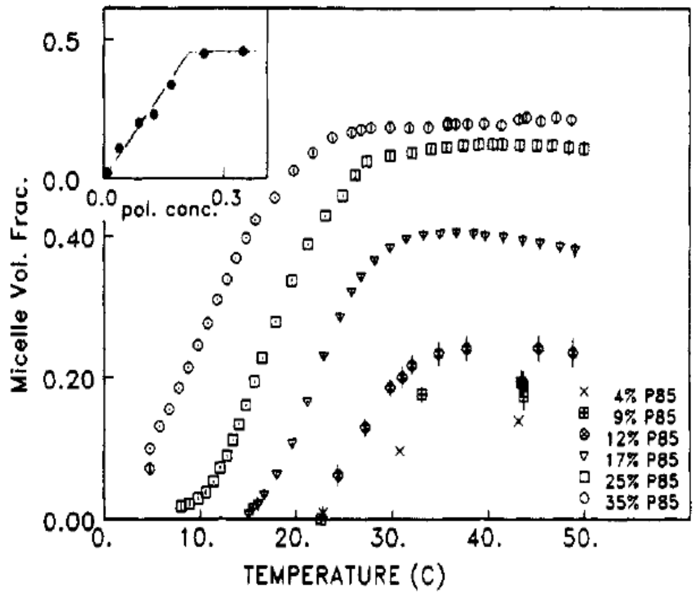
Micellar parameters
as a function of temperature and concentration, obtained from fitting to the scattering data

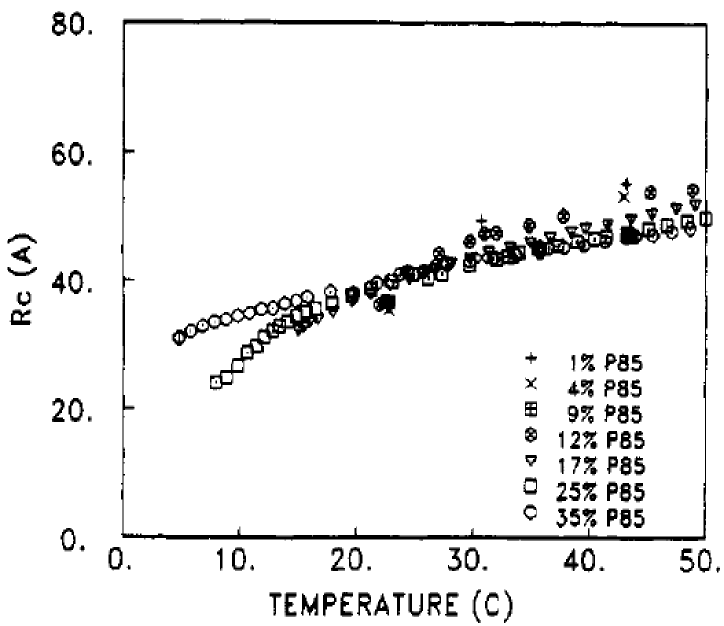
$I(q) = P(q)\,S(q)$

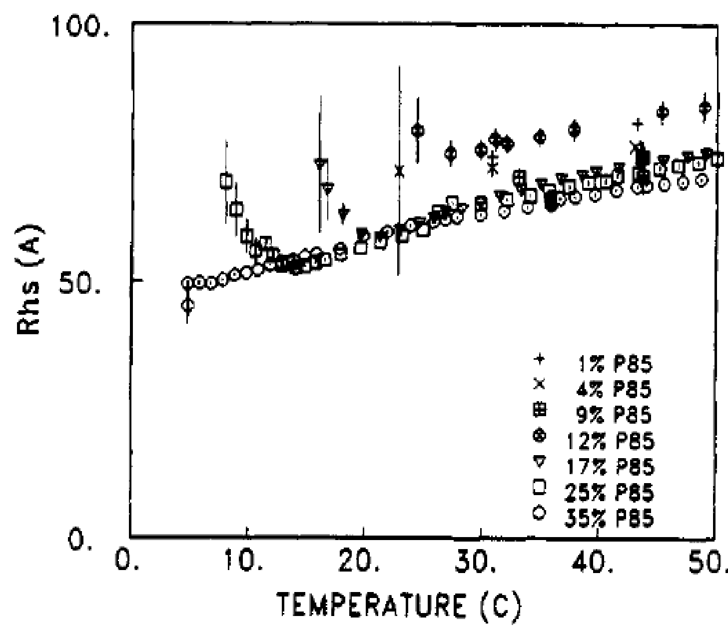
$P(q) = [3(qR_c)^3\{\sin(qR_c)-qR_c\cos(qR_c)\}]^2$

$S(q) = [1 + 24\,f\,G(2qR_{hs})/2qR_{hs}]^{-1}$

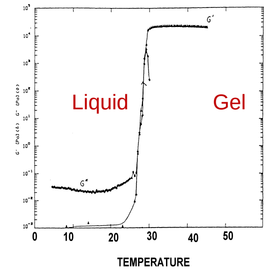
i.e. $I(q)$ function of R_c, R_{hs} and f

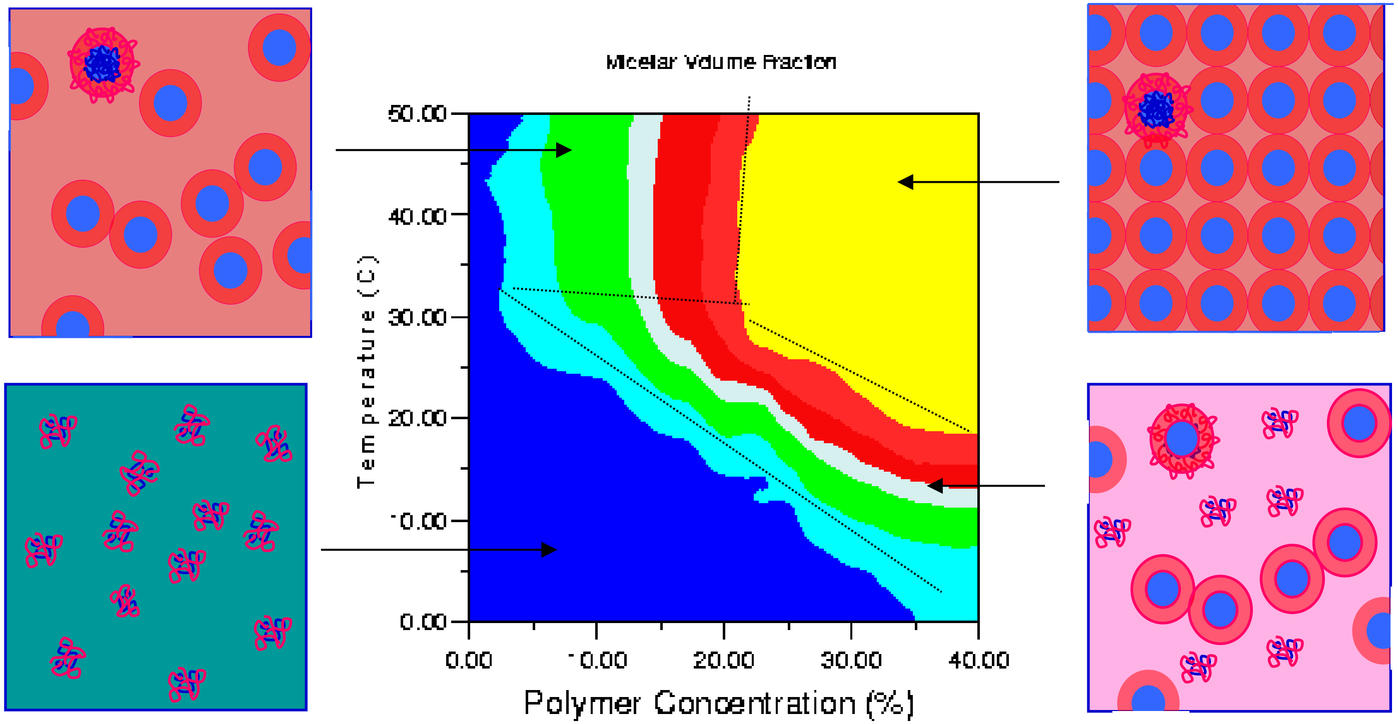






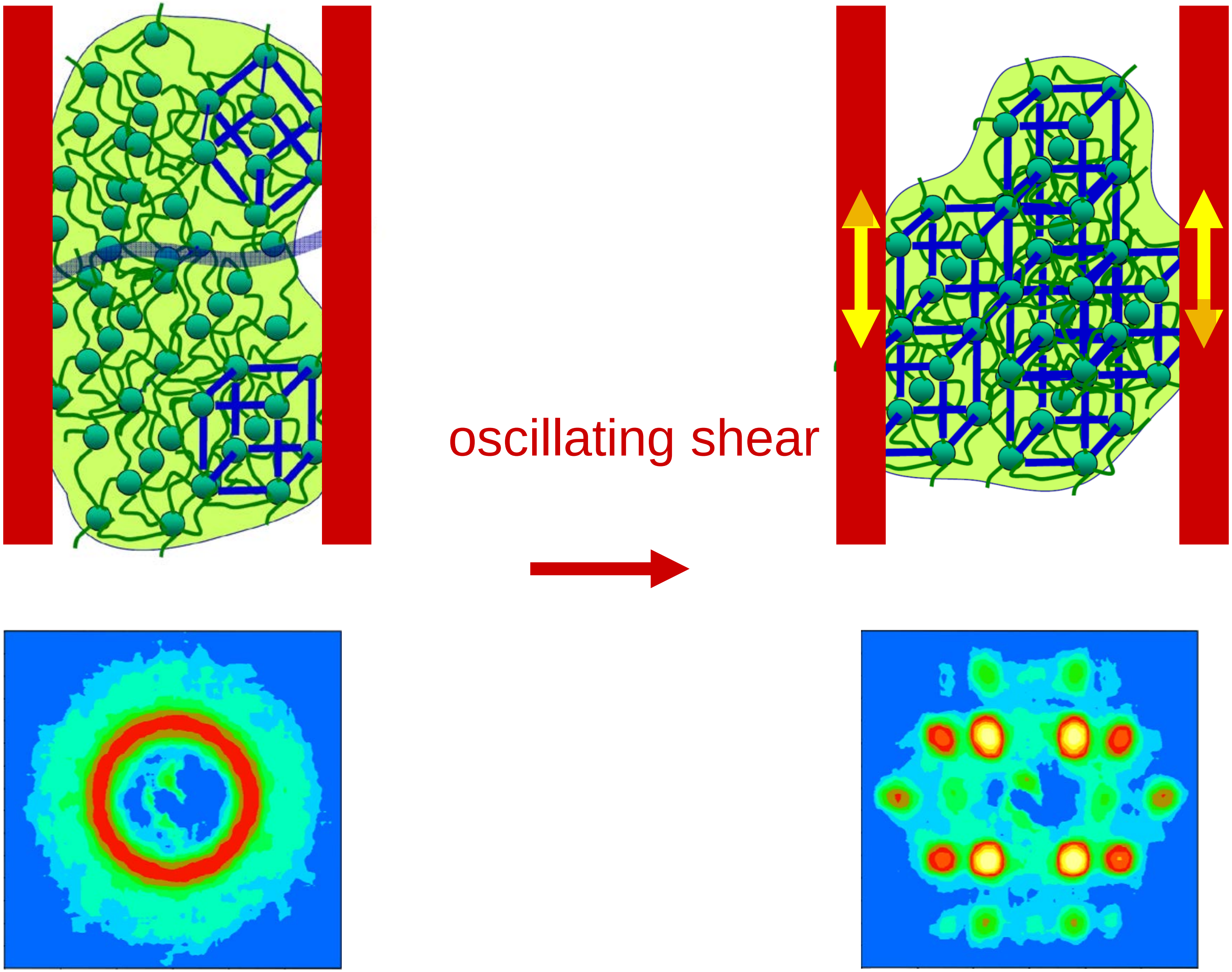
PEO-PPO-PEO Block copolymer in water

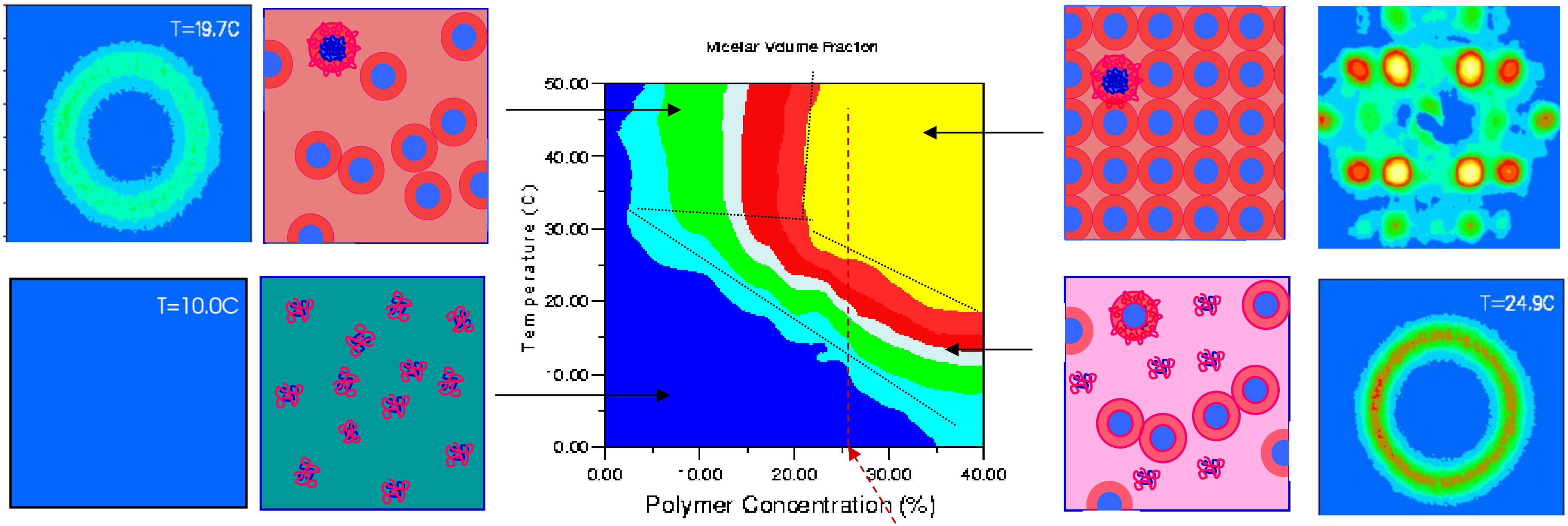




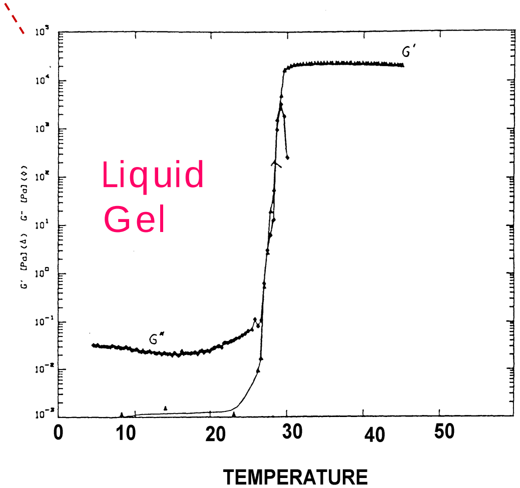
Experimental micellar volume fraction, as obtained from SANS data, and schematic interpretation.
(K.Mortensen. J.Phys.Cond.Matter. 1996)

Orientation by oscillating shear

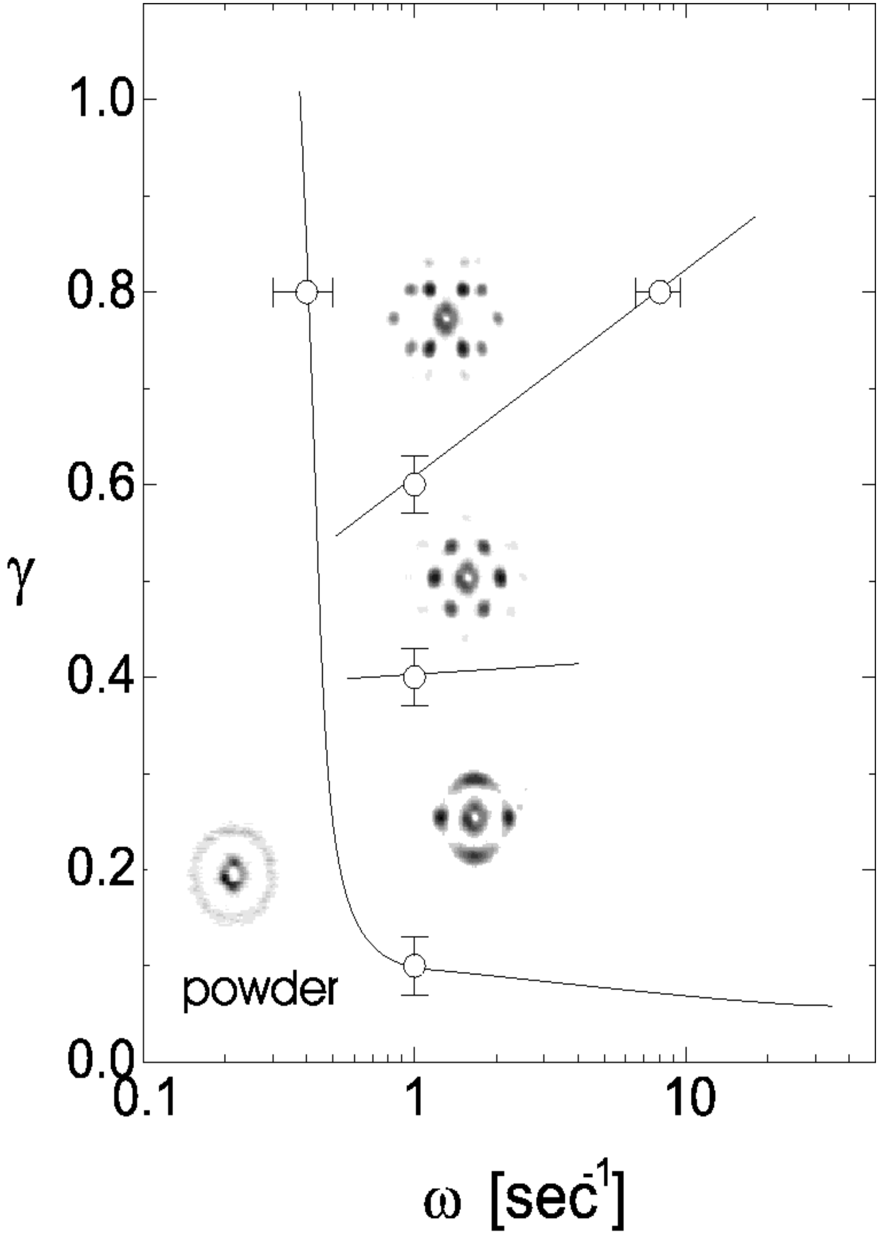




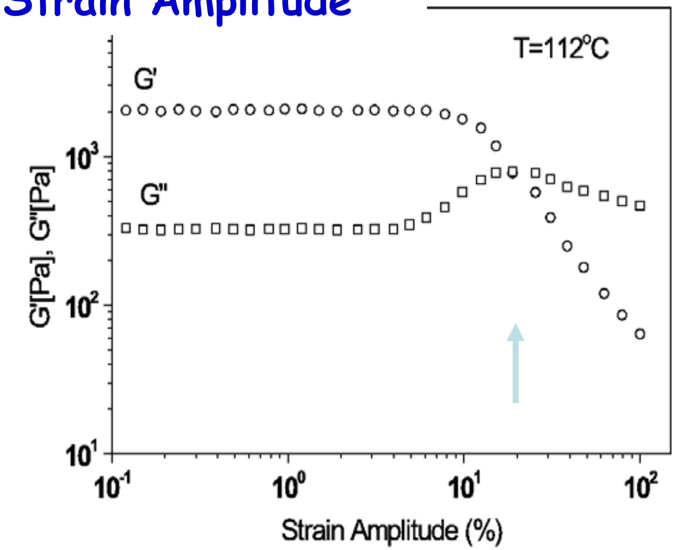
Experimental scattering function
resulting micellar volume fraction,
and
schematic real-space interpretation.
(KM J.Phys.Cond.Matter. 1996)



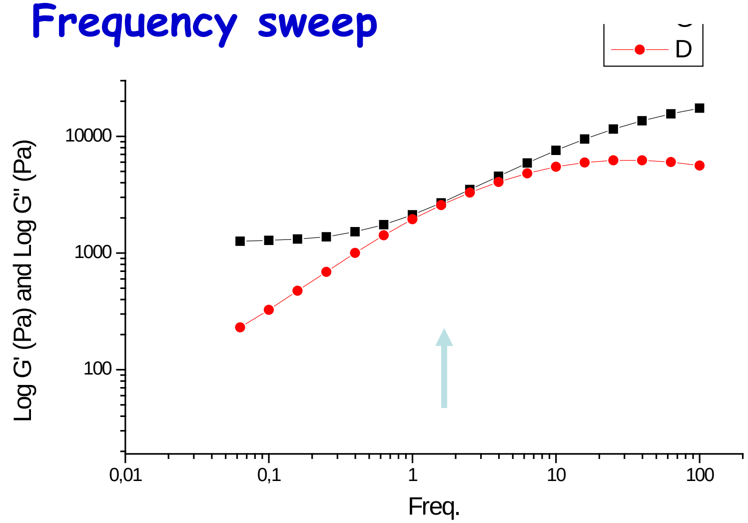
Shear-controlled texture



Strain Amplitude



Frequency sweep



Mortensen et al Macromolecules 2002