Non-particulate 2-phase systems.

(See Roe Sects 5.3, 1.6)

Remember:

$$I(\mathbf{q}) = \int \Gamma_\rho(\mathbf{r}) \, exp(-i\mathbf{qr}) \, d\mathbf{r}$$

In this form, integral does not converge. So

deviation from the mean <n> = $\eta(\mathbf{r}) = \rho(\mathbf{r}) - \langle n \rangle$

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Then

$$\Gamma_\eta(\mathbf{r}) = \int \eta(\mathbf{u})\, \eta(\mathbf{u} + \mathbf{r})\, d\mathbf{u}$$

$$\Gamma_\rho(\mathbf{r}) = \int (\eta(\mathbf{u}) + <\rho>)\, (\eta(\mathbf{u} + \mathbf{r}) + <\rho>)\, d\mathbf{u}$$

Non-particulate 2-phase systems.

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$$+ <\rho> \underbrace{\int \eta(\mathbf{u} + \mathbf{r})\, d\mathbf{u}}_{0}$$

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$$+ <\rho> \int \eta(\mathbf{u} + \mathbf{r})\, d\mathbf{u}$$

0   0

$$\Gamma_\rho(\mathbf{r}) = \Gamma_\eta(\mathbf{r}) + <\rho>^2 V$$

volume of specimen

Non-particulate 2-phase systems.

deviation from the mean $<\rho>$ = $\eta(\mathbf{r}) = \rho(\mathbf{r}) - <\rho>$

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$$+ <\rho> \int \eta(\mathbf{u} + \mathbf{r})\, d\mathbf{u}$$

0

0

$$\Gamma_\rho(\mathbf{r}) = \Gamma_\eta(\mathbf{r}) + <\rho>^2 V$$

leads to null scattering

Non-particulate 2-phase systems.

Finally

$$\Gamma_\rho(\mathbf{r}) = \Gamma_\eta(\mathbf{r})$$

$$I(\mathbf{q}) = \int \Gamma_\eta(\mathbf{r}) \exp(-i\mathbf{q}\mathbf{r})\, d\mathbf{r}$$

Normalization of $\Gamma_\eta(\mathbf{r})$:

$$\gamma(\mathbf{r}) = \Gamma_\eta(\mathbf{r}) / \Gamma_\eta(0)$$

where

$$\Gamma_\eta(0) = \int \eta(\mathbf{u})\, \eta(\mathbf{u} + 0)\, d\mathbf{u} = \langle\eta^2\rangle V$$

Then:

$$I(\mathbf{q}) = \langle\eta^2\rangle V \int \gamma(\mathbf{r})\, \exp(-i\mathbf{q}\mathbf{r})\, d\mathbf{r}$$

Non-particulate 2-phase systems.

$$I(\mathbf{q}) = \langle\eta^2\rangle V \int \gamma(\mathbf{r})\ \exp(-i\mathbf{qr})\ d\mathbf{r}$$

Remember the invariant (total scattering power of specimen):

$$Q = \int I(\mathbf{S})\ d\mathbf{S} = (1/(2\pi)^3) \int I(\mathbf{q})\ d\mathbf{q}$$

= total scattering over the whole of reciprocal space

For isotropic material:

$$Q = 4\pi \int_o^\infty S^2\ I(S)\ dS = (1/(2\pi^2)) \int_o^\infty q^2\ I(q)\ dq$$

$$(S = (2 \sin \theta)/\lambda = q/2\pi)$$

Non-particulate 2-phase systems.

For isotropic material:

$$Q = 4\pi \int_o^\infty S^2\, I(S)\, dS = (1/(2\pi^2)) \int_o^\infty q^2\, I(q)\, dq$$

$$Q = \int \Gamma_\eta(\mathbf{r}) \left[(1/(2\pi^2)) \int exp(-i\mathbf{qr})\, d\mathbf{q} \right] d\mathbf{r} = \Gamma_\eta(0) = \langle \eta^2 \rangle V$$

Non-particulate 2-phase systems.

Now for the model -

Ideal 2-phase system:

- only 2 regions or phases
- each phase has constant scattering length density
- sharp phase boundary
- randomly mixed
- isotropic

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Now for the model -

Ideal 2-phase system:

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sharp phase boundary

randomly mixed

isotropic

Can get:

volume fractions ϕ_i of each phase & interface area

Non-particulate 2-phase systems.

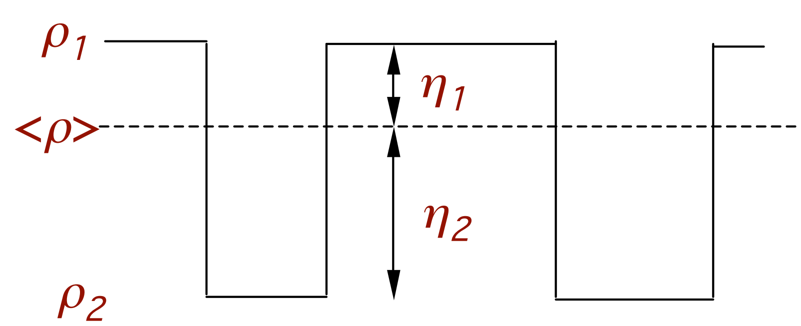
Ideal 2-phase system:

$$\langle\rho\rangle = \phi_1\,\rho_1 + \phi_2\,\rho_2$$

$$\eta_1 = \rho_1 - \langle\rho\rangle = \Delta\rho\,\phi_2$$

$$\eta_2 = \rho_2 - \langle\rho\rangle = \Delta\rho\,\phi_1$$

$$\Delta\rho = \rho_1 - \rho_2 = \eta_1 + \eta_2$$



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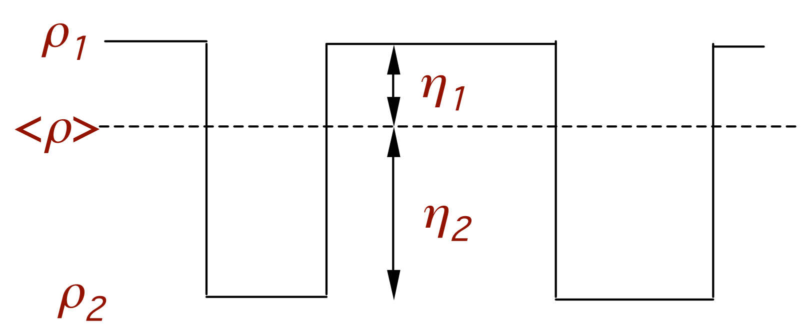


$$Q = \langle\eta^2\rangle V = V\,(\Delta\rho)^2\, \phi_1\phi_2$$

if ρ_1, ρ_2 known, $Q \dashrightarrow \phi_1, \phi_2$

if ϕ_1, ϕ_2 known, $Q \dashrightarrow \rho_1 - \rho_2$

Non-particulate 2-phase systems.

Ideal 2-phase system:

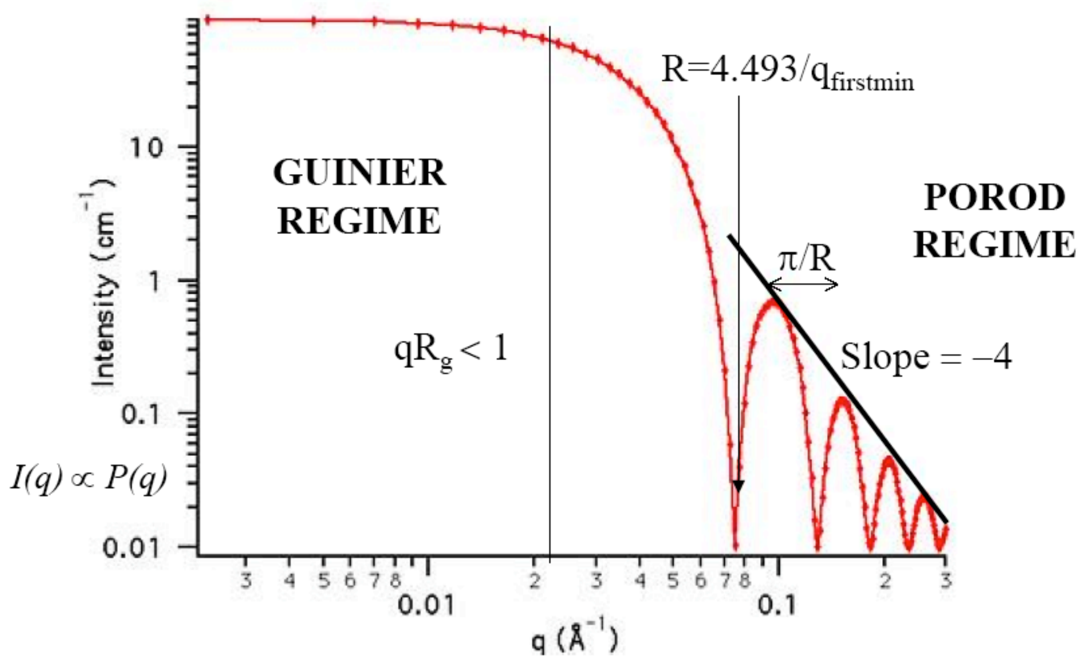
Most important result - Porod law:

$I(q) \rightarrow (2\pi\,(\Delta\rho)^2\,S)/q^4$ at large q

S = total boundary area betwn 2 phases

$\log I(q) = const - 4 \times \log q$

Dilute monodisperse spheres



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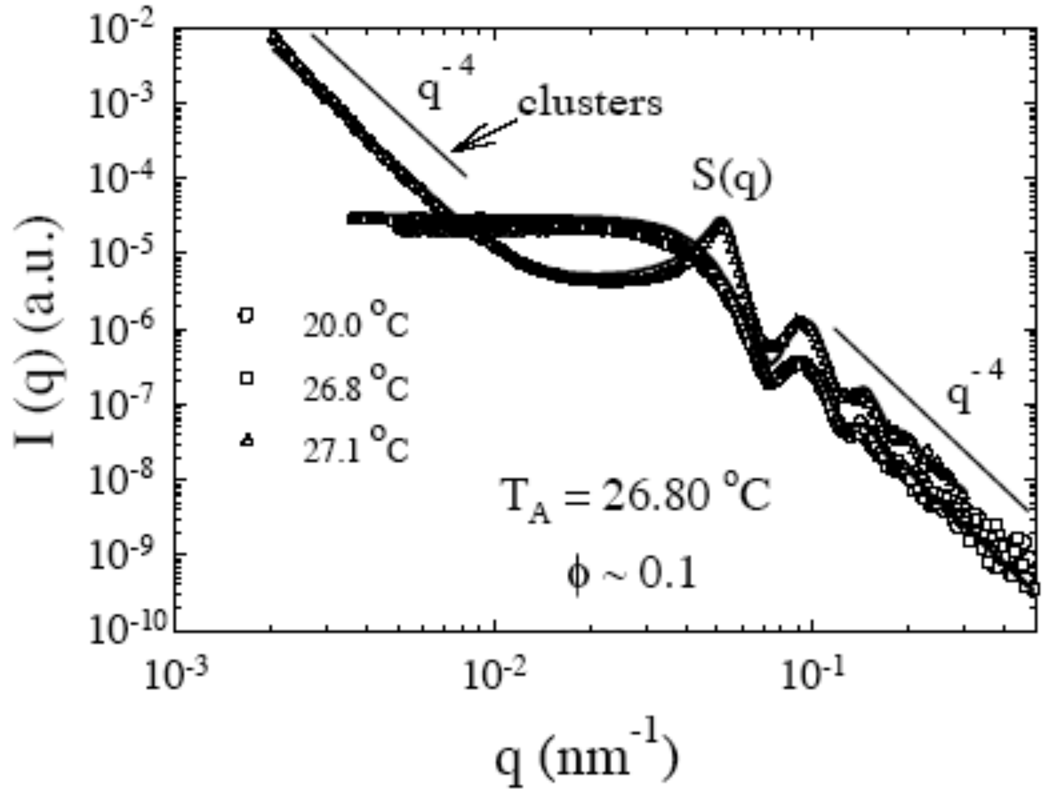

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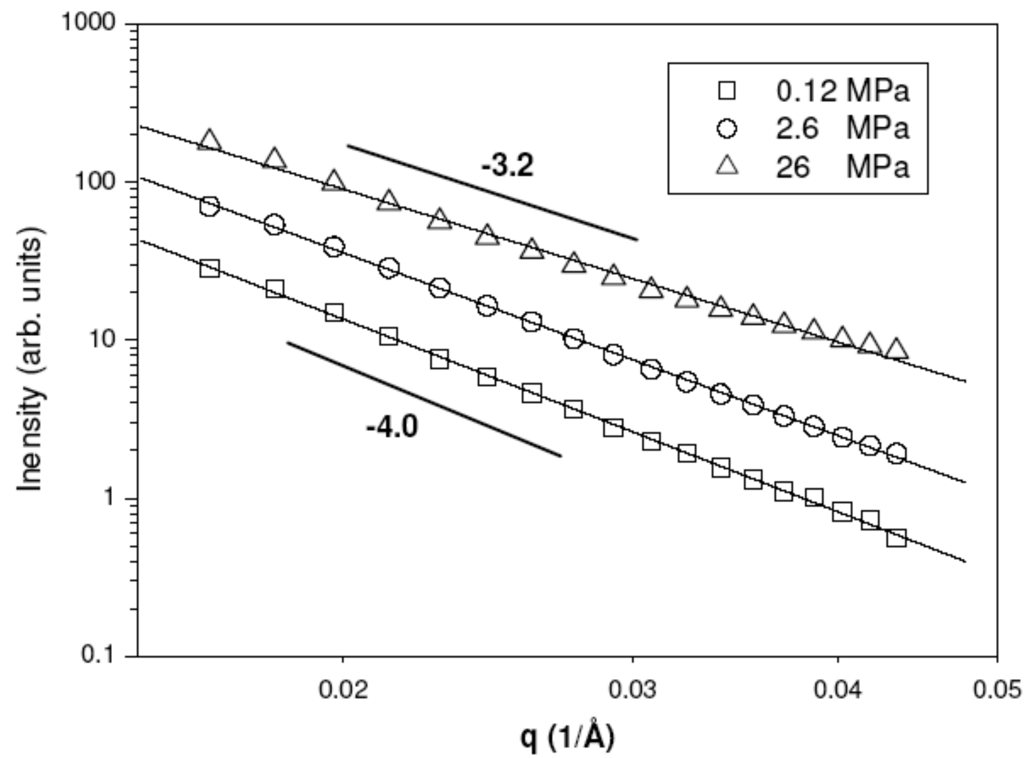
Need absolute Is

If relative Is, can get invariant $Q \text{ --> } S/V$

$I(q)/Q = (2\pi S)/(\phi_1 \phi_2 V q^4)$



Non-particulate 2-phase systems.

Deviations from ideal 2-phase system

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Density fluctuations (from thermal motion):

$$I(q) = I_o(q) + I_1(q) + I_2(q) + I_{12}(q)$$

uniform density (I_o) density fluctuations (I_1, I_2) interaction betwn phases (I_{12})

Non-particulate 2-phase systems.

Deviations from ideal 2-phase system

$$I(q) = I_o(q) + I_1(q) + I_2(q) + I_{12}(q)$$

uniform density ($I_o(q)$)

density fluctuations ($I_1(q)$, $I_2(q)$)

= intensity from pure phases
weighted by vol %s

interaction betwn phases ($I_{12}(q)$)

short range correlations -
small, neglected

Non-particulate 2-phase systems.

Deviations from ideal 2-phase system

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uniform density → $I_o(q)$

density fluctuations → $I_1(q)$, $I_2(q)$

interaction betwn phases → $I_{12}(q)$

density fluctuations = intensity from pure phases weighted by vol %s

interaction betwn phases: short range correlations - small, neglected

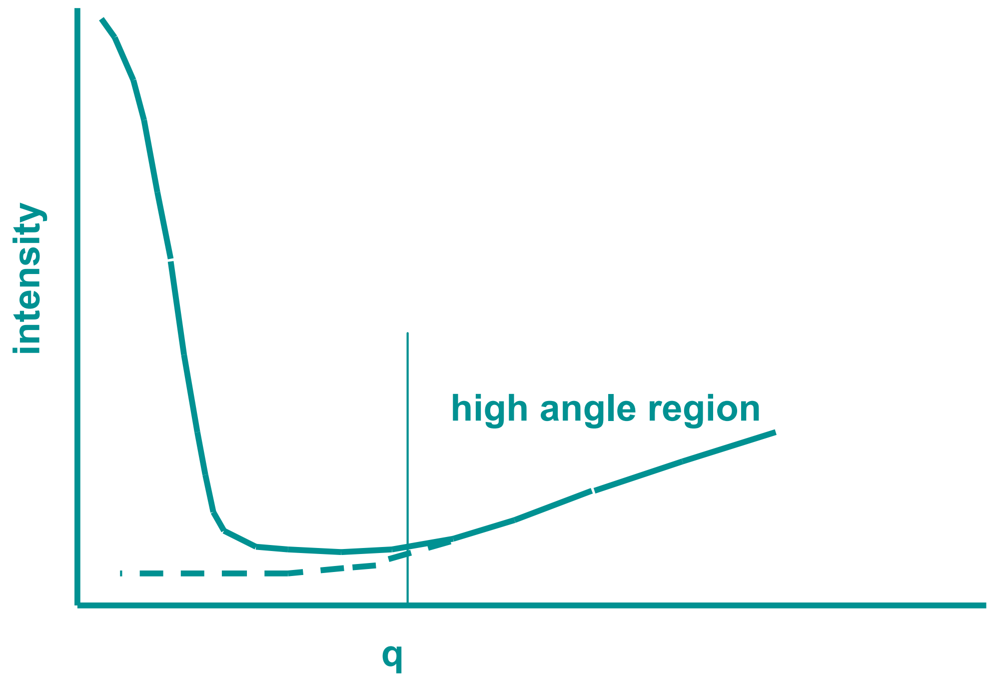
To correct, then, measure scattering from the 2 pure phases

Non-particulate 2-phase systems.

Deviations from ideal 2-phase system

Al otro lado:

can make empirical correction for $I_1(q) + I_2(q)$



Non-particulate 2-phase systems.

Deviations from ideal 2-phase system

Diffuse boundary betwn phase regions:

let $\rho(\mathbf{r})$ = scattering length density in 2-phase matl w/ diffuse boundaries

$\rho_{id}(\mathbf{r})$ = scattering length density in the same 2-phase matl w/ sharp boundaries (hypothetical)

Non-particulate 2-phase systems.

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Then

$$\rho(\mathbf{r}) = \rho_{id}(\mathbf{r}) * g(\mathbf{r})$$

$g(\mathbf{r})$ = fcn which characterizes diffuse boundaries

Non-particulate 2-phase systems.

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$I(\mathbf{q}) = I_{id}(\mathbf{q})\, G^2(\mathbf{q})$ $\quad$ $G(\mathbf{q})$ = Fourier transform of $g(\mathbf{r})$

(Fourier transform of convolution of 2 fcns = product of their transforms)

Non-particulate 2-phase systems.

Deviations from ideal 2-phase system

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(Fourier transform of convolution of 2 fcns = product of their transforms)

Common:

$G(\mathbf{q}) = exp(-\sigma^2/2)q^2$ & for small bdy width (σ):

$I(\mathbf{q}) = I_{id}(\mathbf{q})\,(1 - \sigma^2\, q^2)$

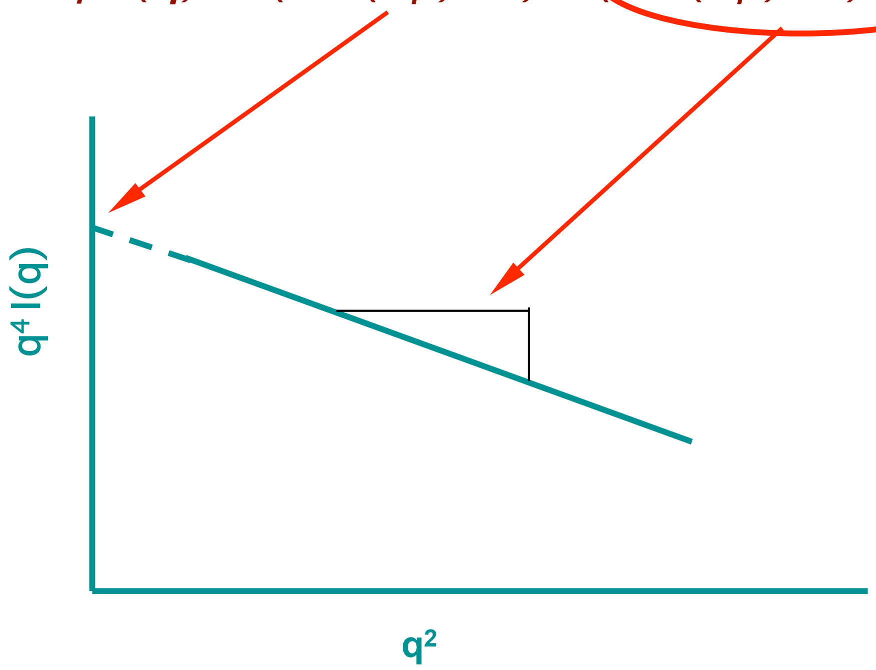
Non-particulate 2-phase systems.

Deviations from ideal 2-phase system

Diffuse boundary betwn phase regions:

$$I(q) = I_{id}(q)\ (1 - \sigma^2 q^2)$$

$$q^4 I(q) = (2\pi\ (\Delta\rho)^2 S) - (2\pi\ (\Delta\rho)^2 S)\ (\sigma^2 q^2)$$



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