The Theoretical Foundation of Spin-Echo Small-Angle Neutron Scattering (SESANS) Applied in Colloidal System

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UCANS-II Indiana University
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Bloomington, IN

Outline

1. Motivation

   — why Spin-Echo Small-Angle Neutron Scattering (SESANS)?

2. Basic Theory

   — what does SESANS measure?

3. Results and Discussions

   — what can SESANS do?

(1). Straightforward observation of potential

(2). Sensitivity to the local structure

(3). Sensitivity to the structural heterogeneity

4. Summary

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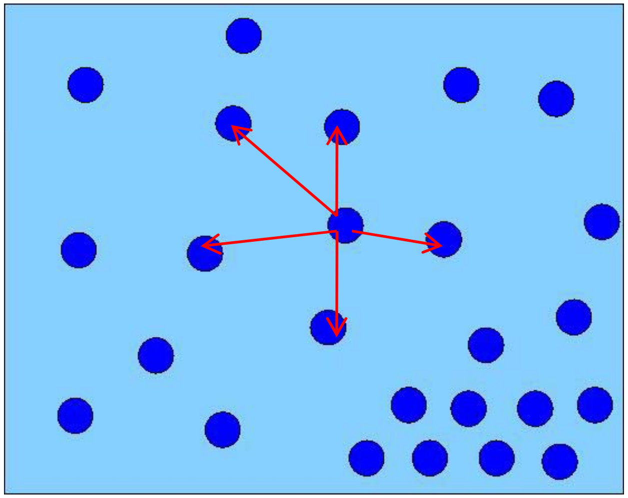
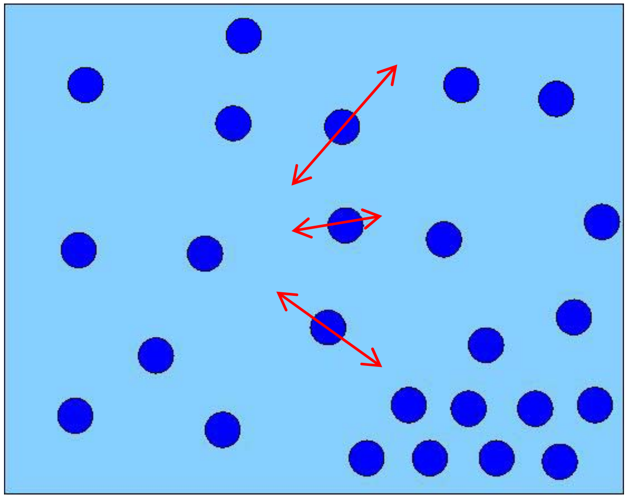
Neutron Scattering

	Structure (Elastic Scatt.)	Dynamics (Inelastic Scatt.)
Unpolarized beam	Small-Angle Neutron Scattering (SANS), Neutron Diffraction, Neutron Reflectometry	Quasi-Elastic Neutron Scattering (QENS), Inelastic Neutron Scattering (INS)
Polarized beam	Spin-Echo Small-Angle Neutron Scattering (SESANS)	Neutron Spin-Echo (NSE)





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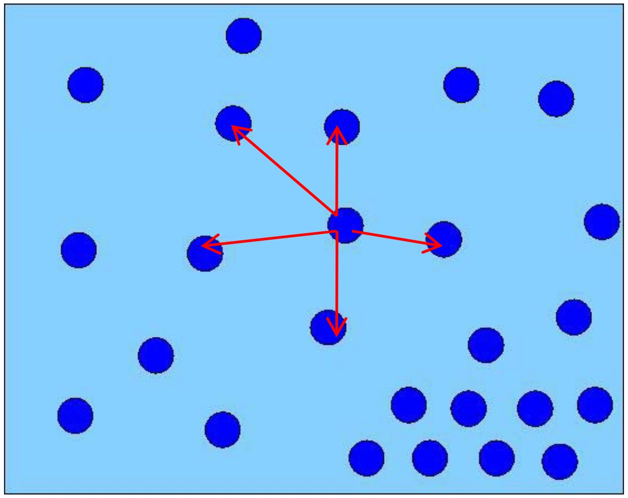
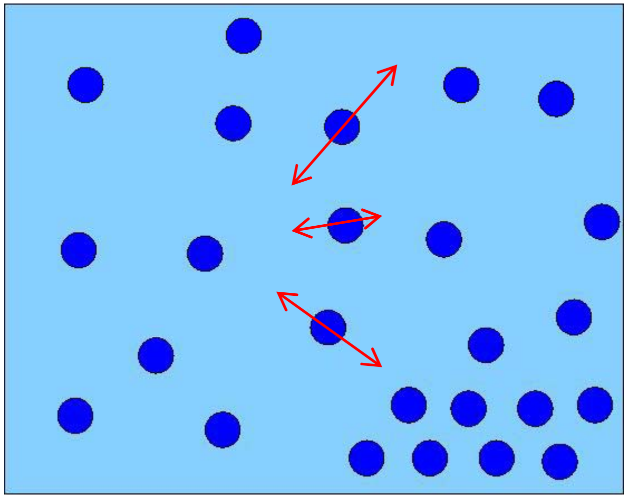
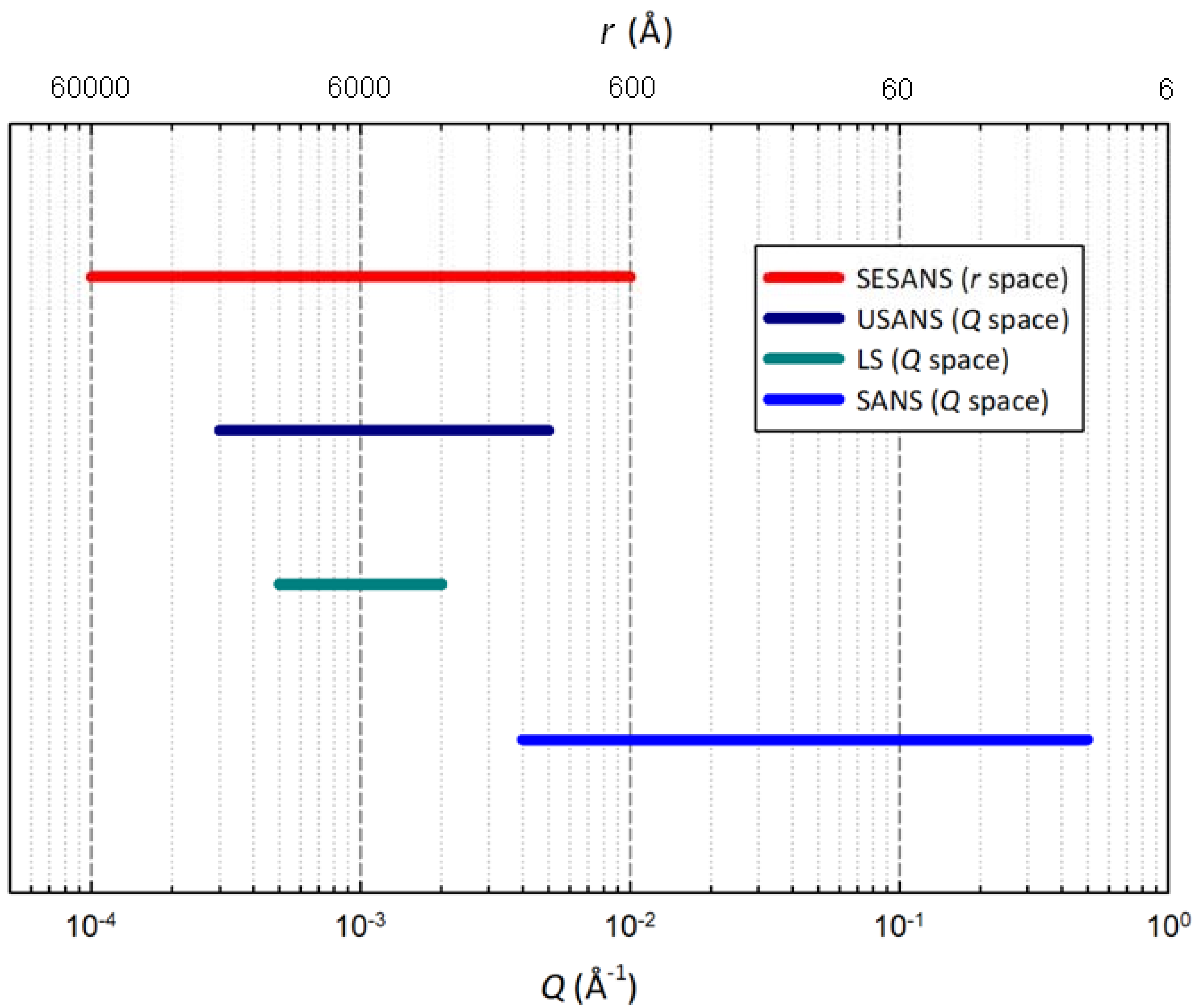




Length scale probed by SESANS



Comparison to other investigation tools

Comparison to Light Scattering

- Extended length scale range
- Multiple scattering
- Transparent samples

Comparison to Ultra-Small Angle Neutron Scattering (USANS)

- Much higher flux

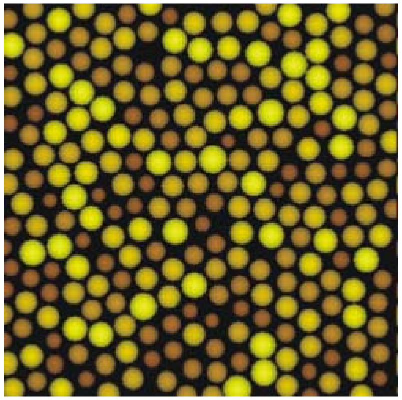
Comparison to Transmission Electron Microscope (TEM)

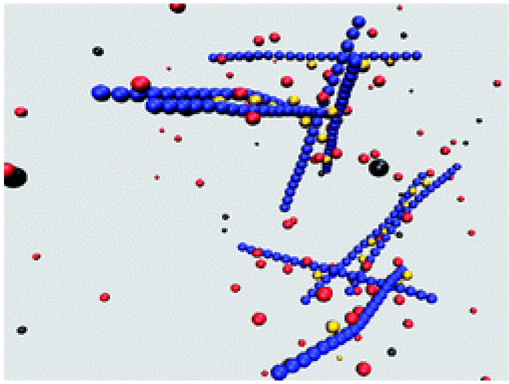
- Non-destructive nature

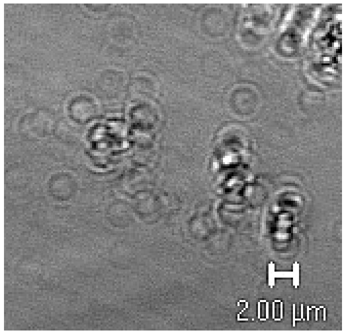
Comparison to Confocal Microscopy

- Ensemble average information

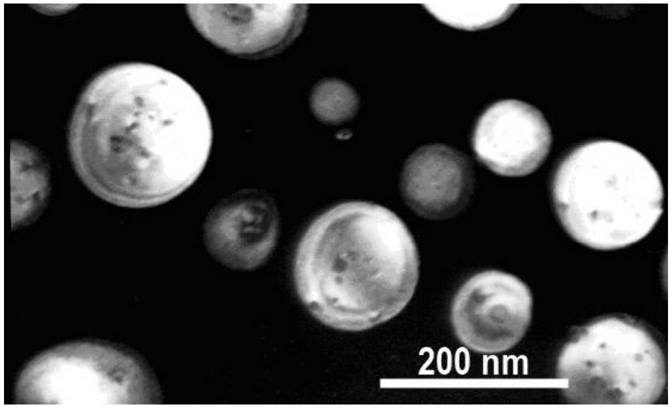
Examples for SESANS







- Highly concentrated systems such as colloidal glass (e.g. PMMA/PS binary glass)
- Large scale structure (polyelectrolyte aggregation) observed in the polyelectrolyte systems (protein, DNA, ionic polymers)
- Optoelectronic soft matters such as polymeric solutions of PLED/OLED
- Precipitate-strengthening superalloy



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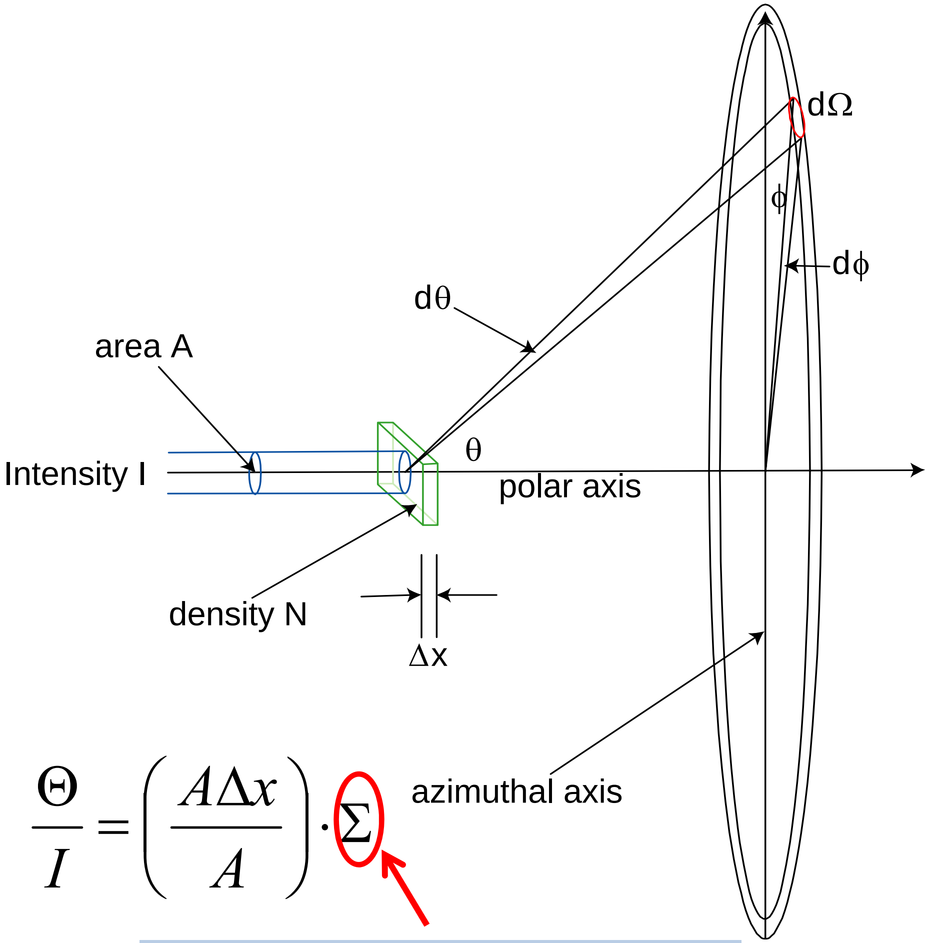
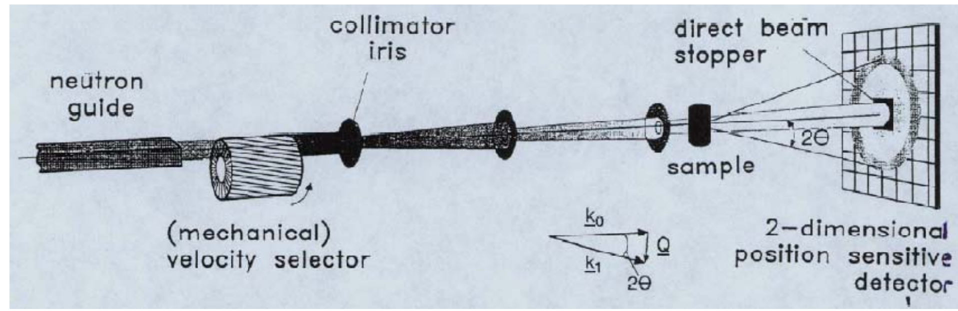
Small Angle Neutron Scattering (SANS)
—measure the structure



$$\frac{\Theta}{I} = \left(\frac{A\Delta x}{A}\right) \cdot \Sigma$$

Scattering cross section



$$I(Q) = \frac{d\Sigma}{d\Omega}(Q)$$

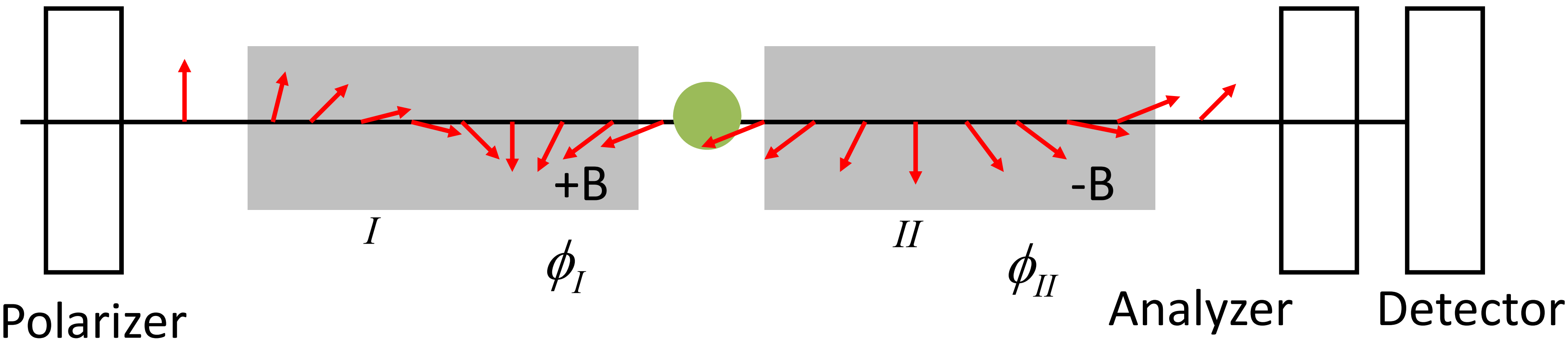
Wave vector $\vec{Q}$

(Momentum transfer)

$$Q = \frac{4\pi}{\lambda}\sin\frac{\theta}{2}$$

Roger Pynn *Small Angle Neutron Scattering*
(http://www.iub.edu/~neutron/)

Neutron Spin Echo (NSE) — measure the dynamics



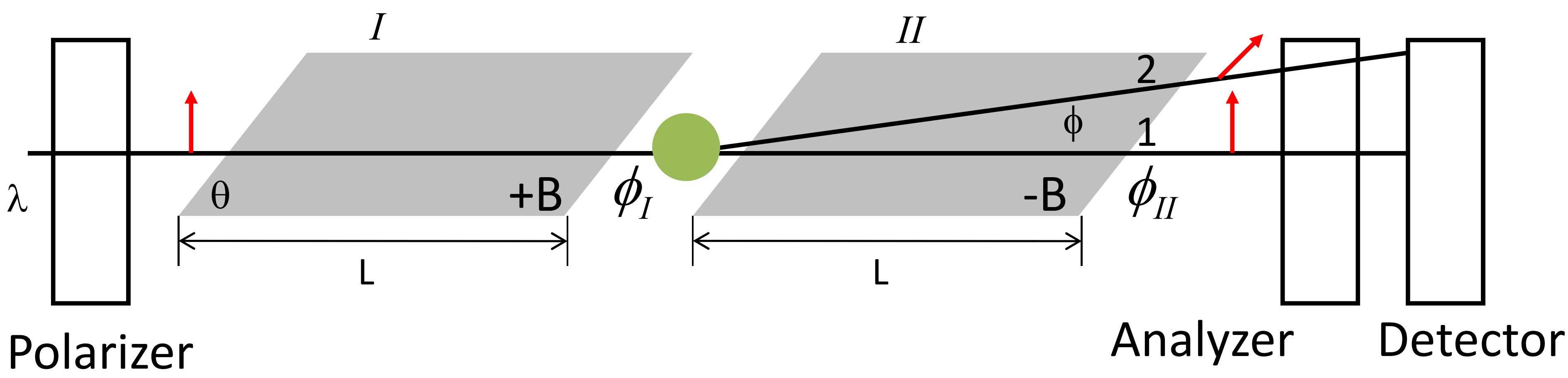
$$P = \int S(Q,\omega)\cos(\phi_{II} - \phi_I)\, d\omega = \int S(Q,\omega)\cos(\omega\tau)\, d\omega = S(Q,\tau)$$

where the "spin echo time" $\tau = \dfrac{cBL\lambda^3 m}{2\pi\hbar}$

$$c = 4.6368\times10^{14}\, T^{-1} m^{-2}$$

Mezei, in *Neutron Spin Echo*, Ed. Mezei, Springer 1980

Spin-Echo Small-Angle Neutron Scattering (SESANS) — measure the structure



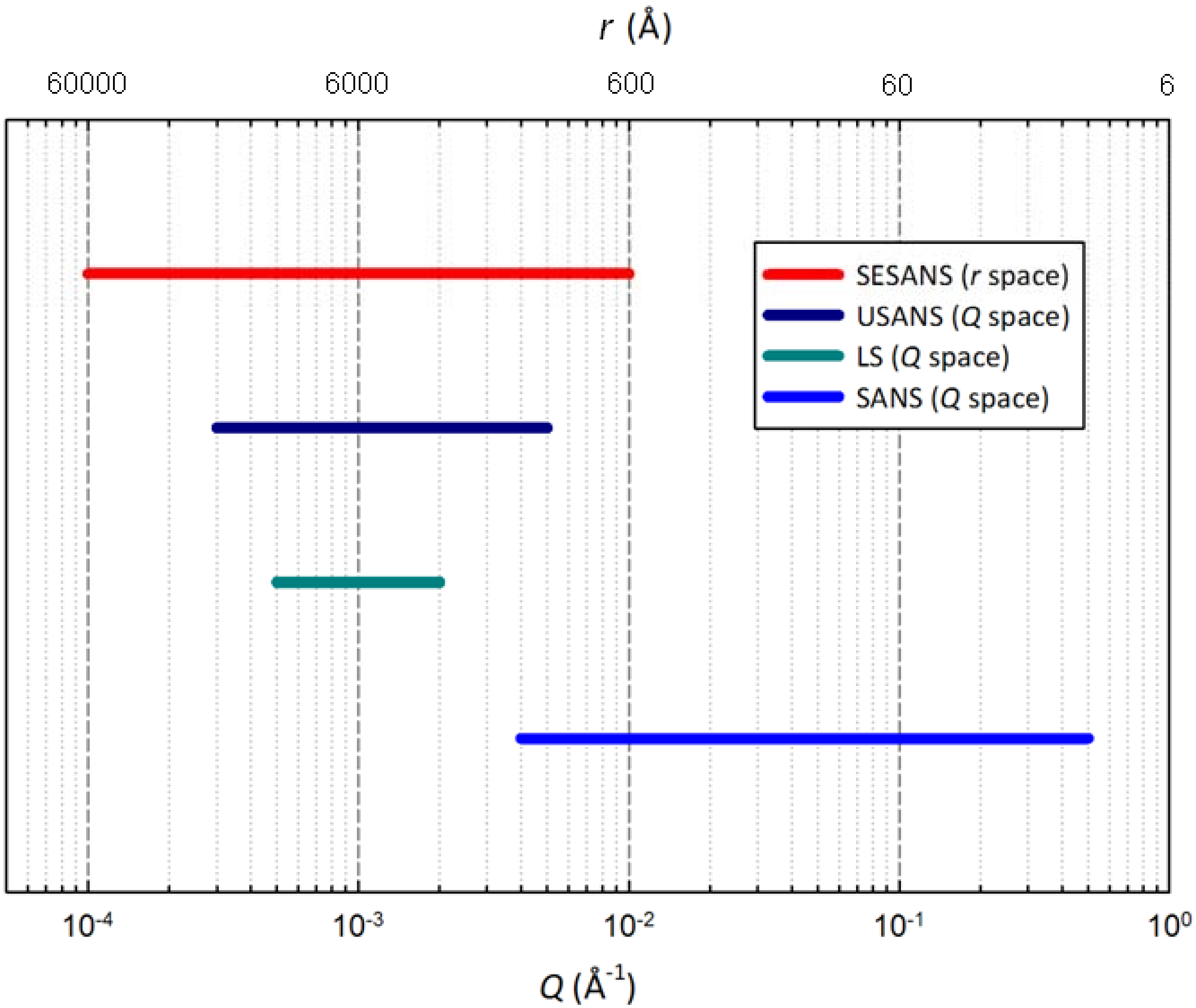
$$P = \int \frac{d\Sigma}{d\Omega}(\vec{Q}) \cos(\phi_{II} - \phi_I)\, d^3\vec{Q} = \int \frac{d\Sigma}{d\Omega}(\vec{Q}) \cos(zQ_z)\, d^3\vec{Q} = G(z)$$

where the "spin echo length" $z = \dfrac{cBL\lambda^2 \cot\theta}{2\pi}$

$$c = 4.6368 \times 10^{14}\, T^{-1} m^{-2}$$

Pynn, *Lecture 11, Neutron Physics and Scattering*
Indiana University (http://www.iub.edu/~neutron/)

Length scale probed by SESANS



Density Profile **Debye Correlation Function**

$$\rho(\vec{r}) \longrightarrow \gamma(r) = \frac{1}{V}\left\langle \int_V \rho(\vec{r'})\rho(\vec{r'}+\vec{r})d^3\vec{r'} \right\rangle$$

SANS

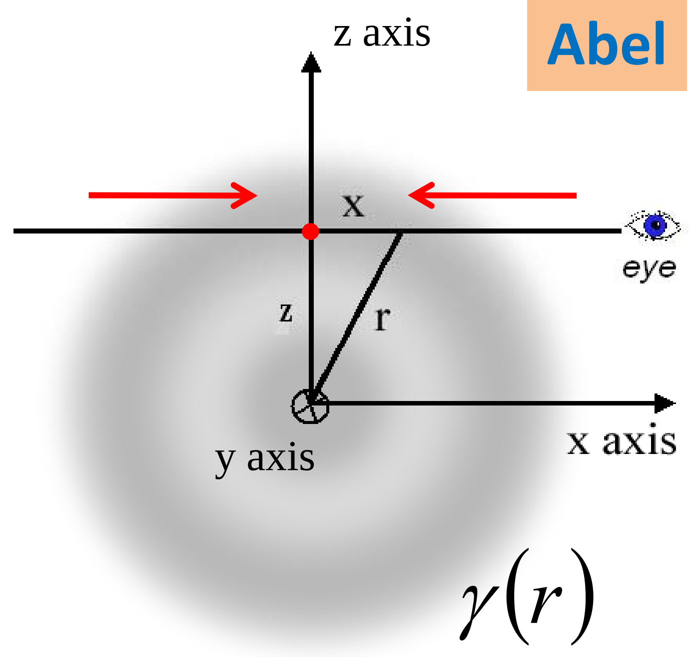
SESANS

$$I(Q) = \frac{d\Sigma}{d\Omega}(Q) = 4\pi\int_0^\infty \gamma(r)J_0(Qr)r^2 dr$$

Fourier

$$G(z) = 2\int_z^\infty \gamma(r)\frac{r}{\sqrt{r^2 - z^2}}dr$$

Abel



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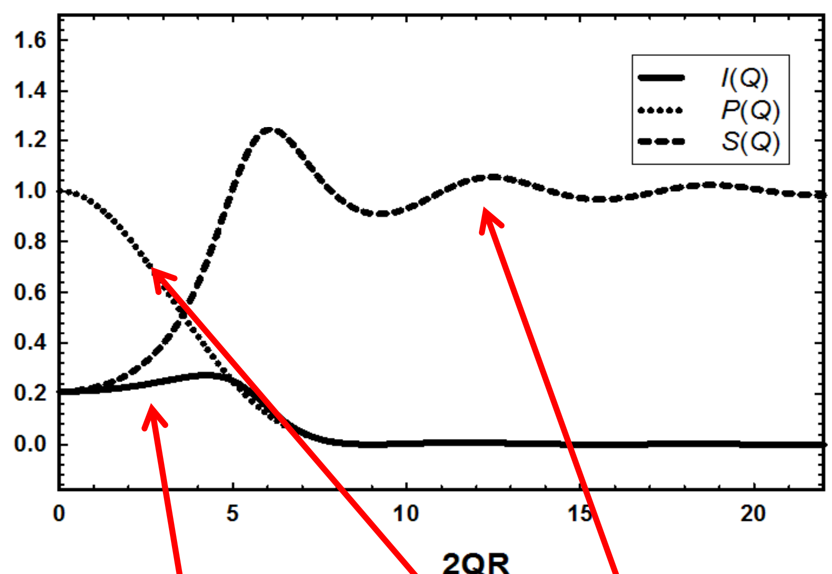
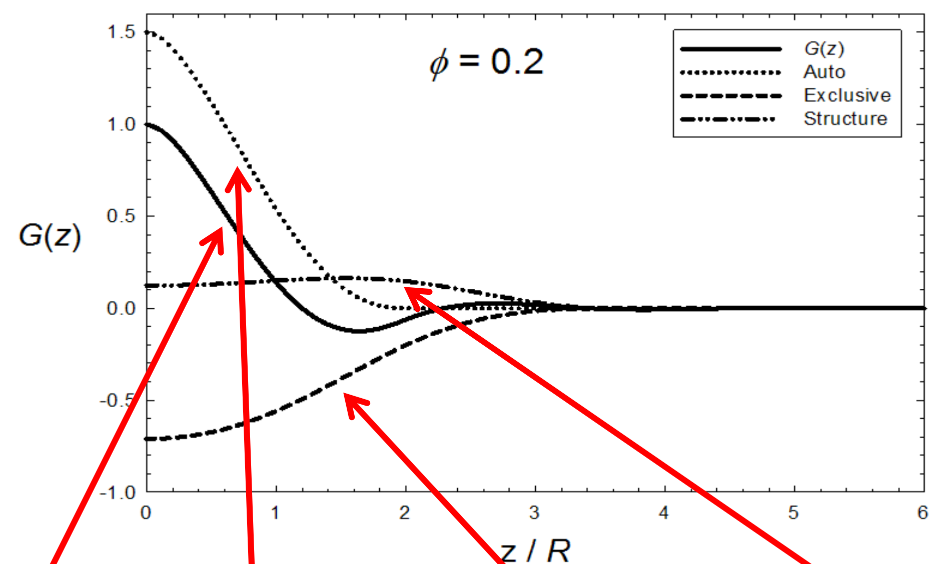
SESANS

$$I(Q) = \frac{d\Sigma}{d\Omega}(Q) = 4\pi\int_0^\infty \gamma(r)J_0(Qr)r^2dr$$

$$G(z) = 2\int_z^\infty \gamma(r)\frac{r}{\sqrt{r^2 - z^2}}dr$$

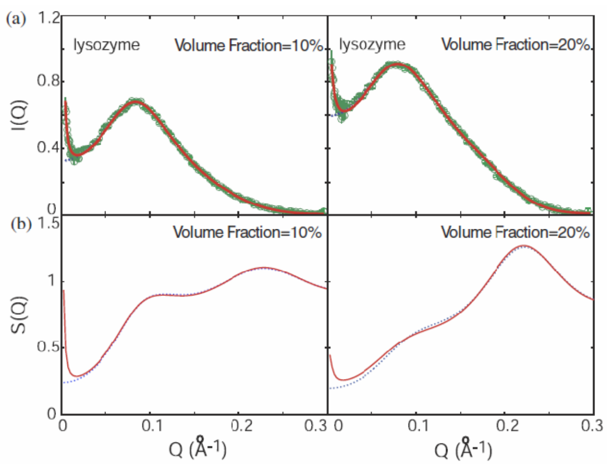




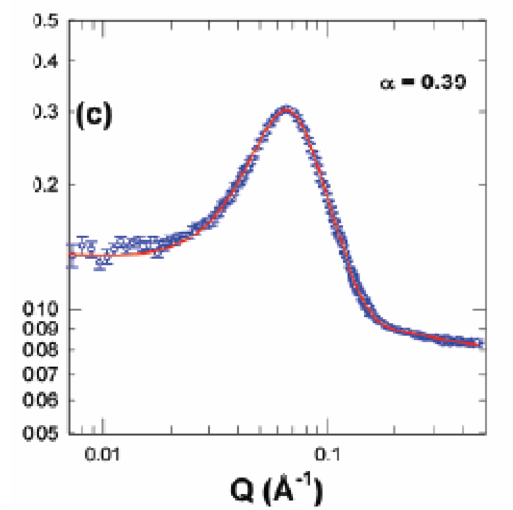
$$I(Q) = nP(Q)S(Q)$$

$$G(z) = G_{auto}(z) - nG_{excl}(z) + nG_{struct}(z)$$

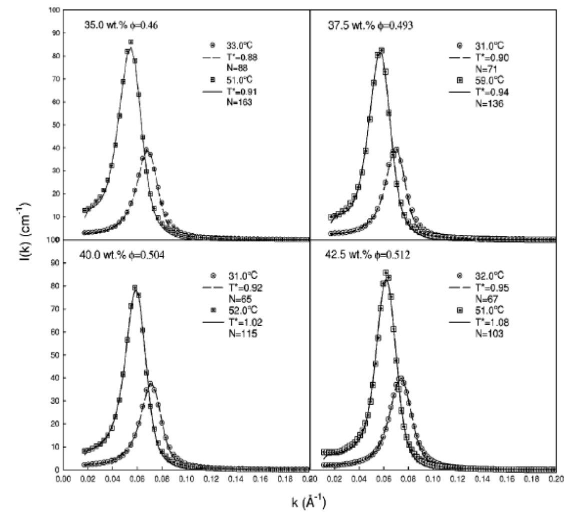
Interaction in concentrated hard colloidal system



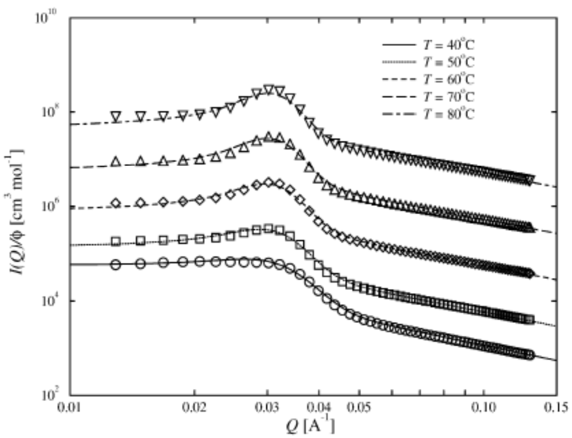
Liu *et al.* PRL **95** 118102 2005



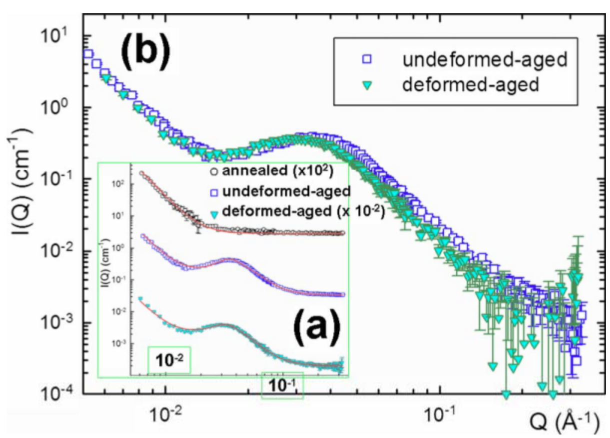
Chen *et al.* Macromolecules **40** 5887 2007



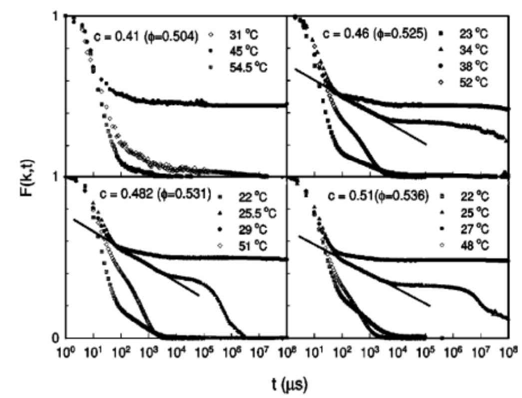
Chen *et al.* Science **300** 619 2003



Likos *et al.* PRE **58** 6229 1998



Huang *et al.* APL **93** 161904 2008



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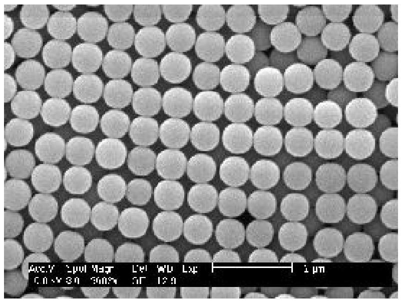
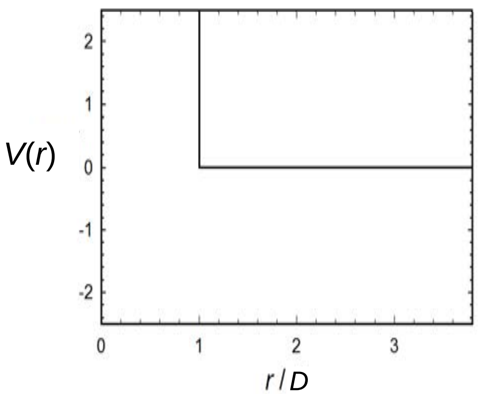
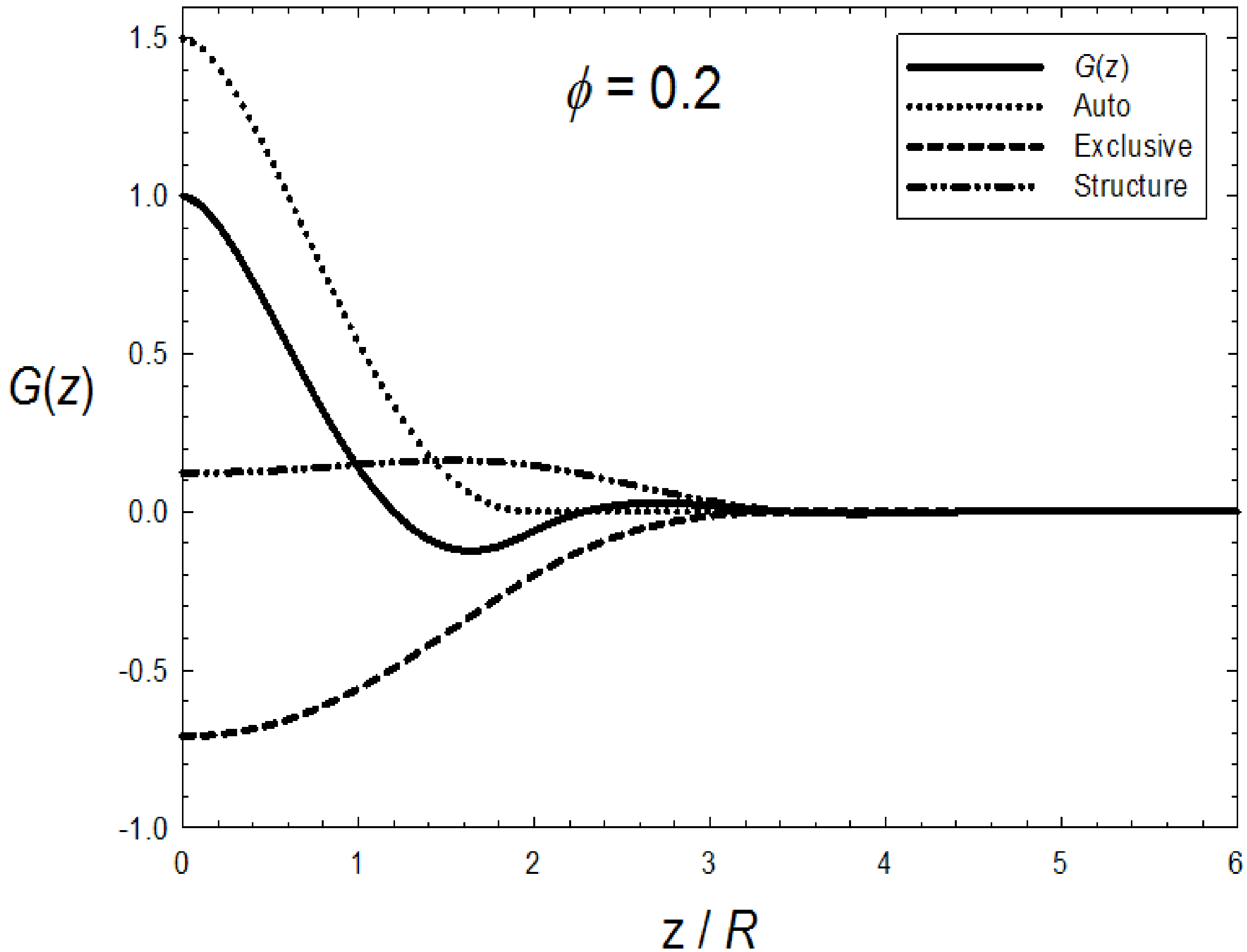
Example I: Hard Sphere Potential



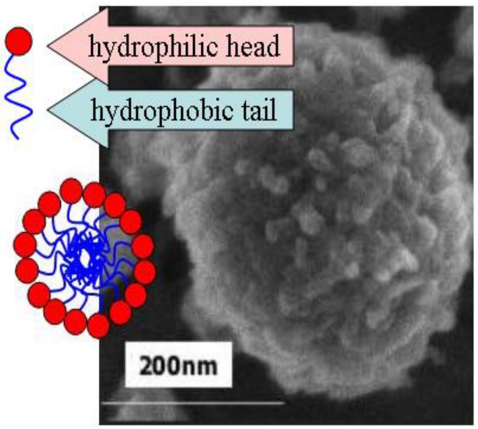
$$V(r) = \begin{cases} \infty & r < D \\ 0 & r > D \end{cases}$$



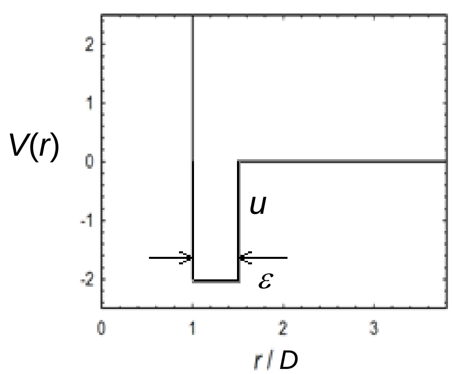


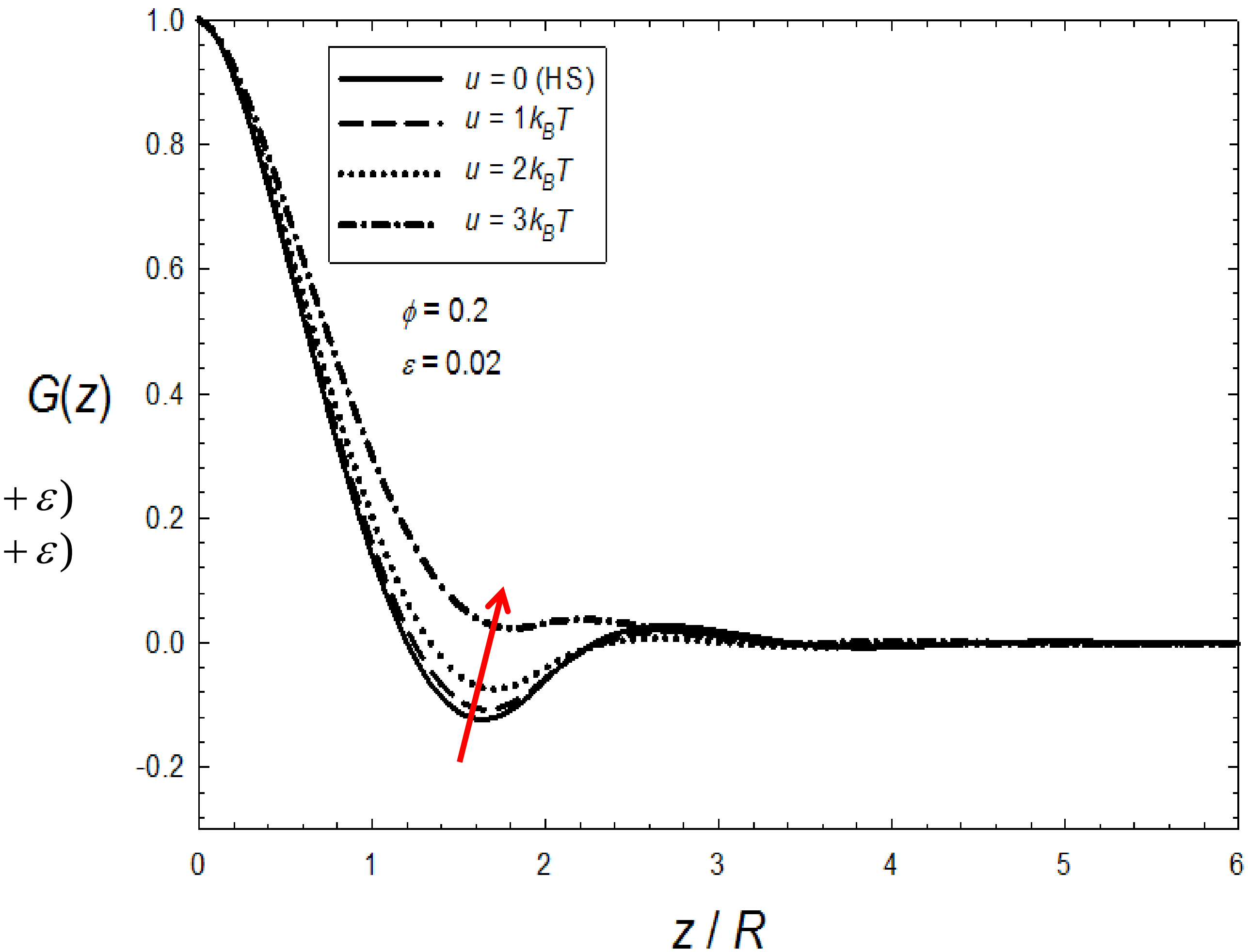
Li *et al., J. Chem. Phys.* **132** 174509 2010

Example II: Attractive Potential



$$V(r)=\begin{cases}\infty & r<D\\ -u & D<r<D(1+\varepsilon)\\ 0 & r>D(1+\varepsilon)\end{cases}$$





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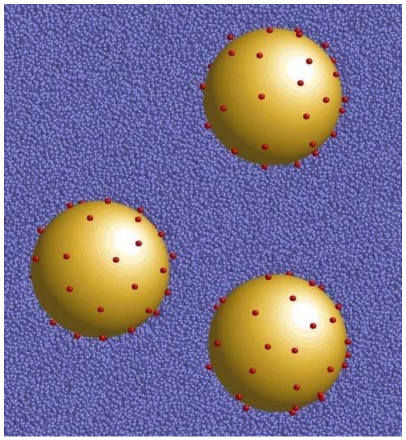
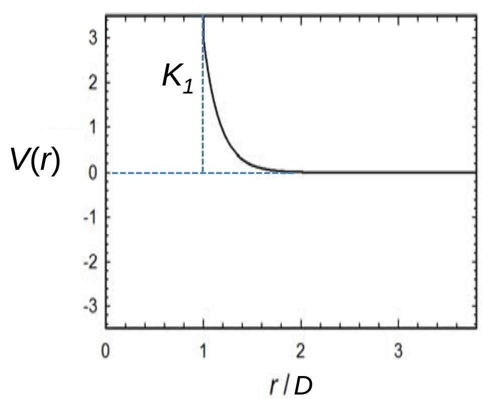
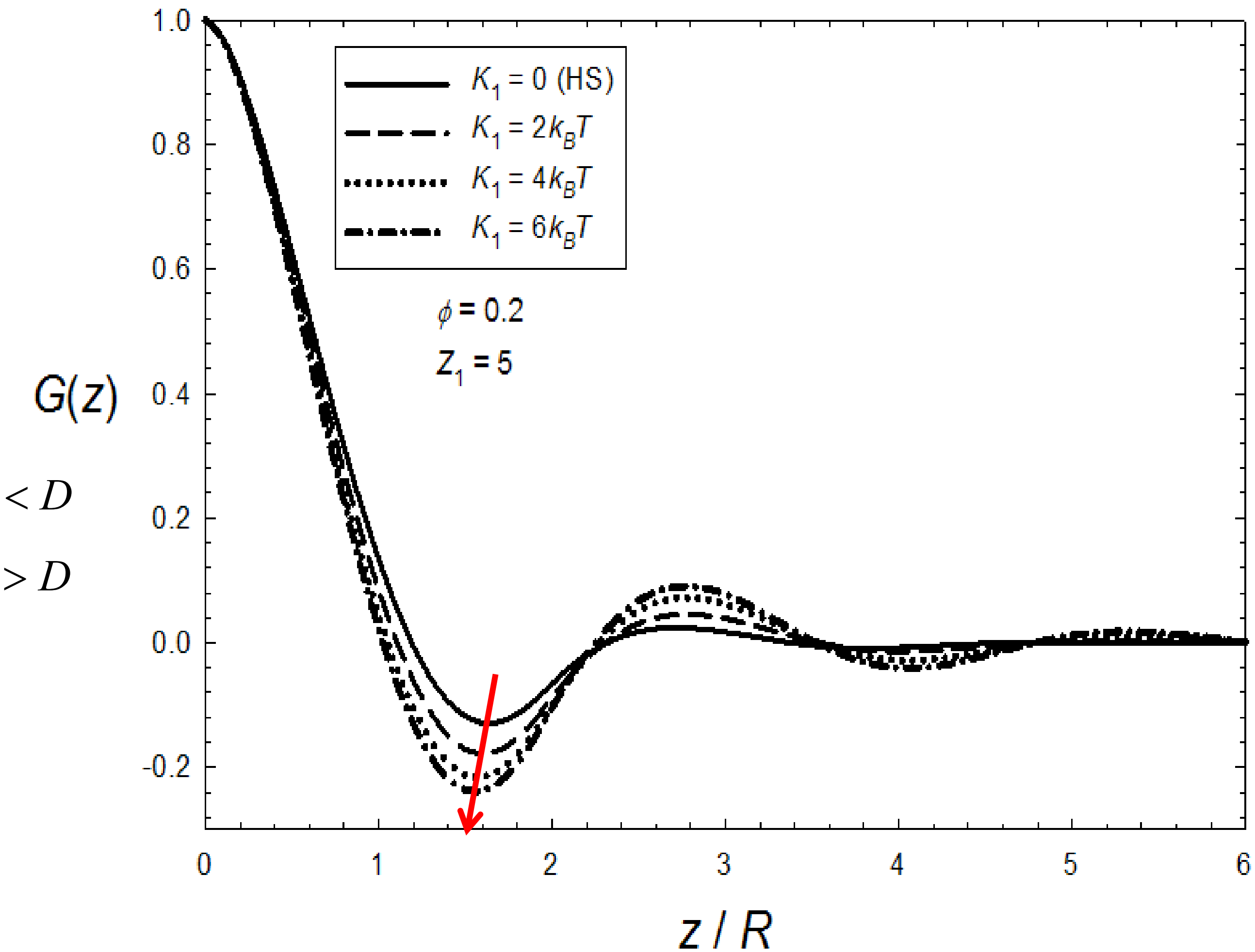
Example III: Screened Coulomb Repulsion Potential



$$V(r) = \begin{cases} \infty & r < D \\ K_1 \dfrac{\exp[-Z_1(r-D)]}{r} & r > D \end{cases}$$





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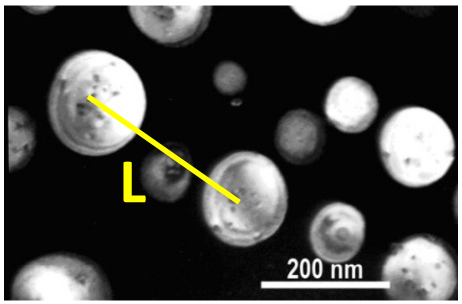
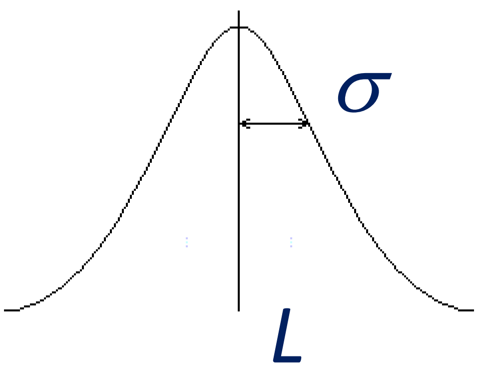
Sensitivity to the local structure



Phenomenological Model



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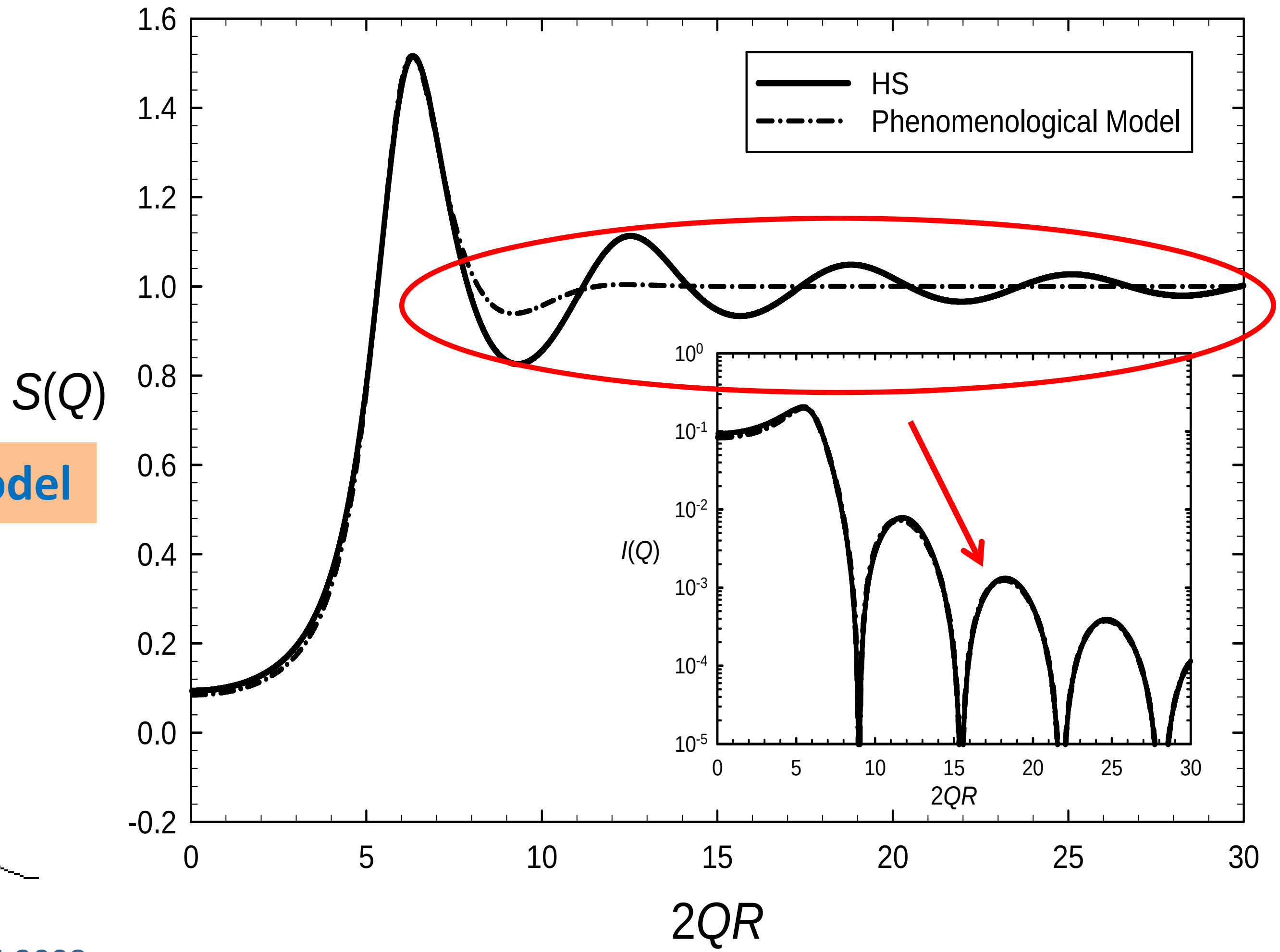

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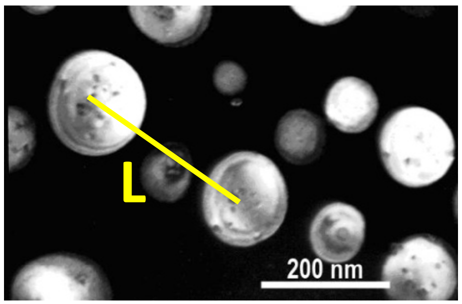
Sensitivity to the local structure



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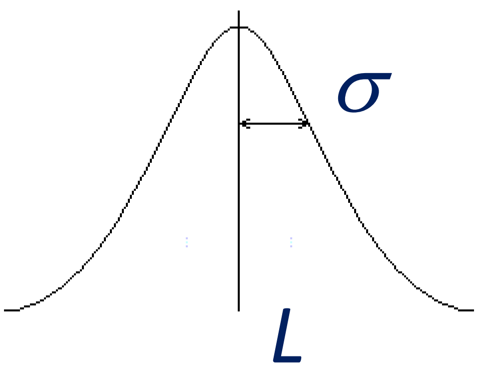

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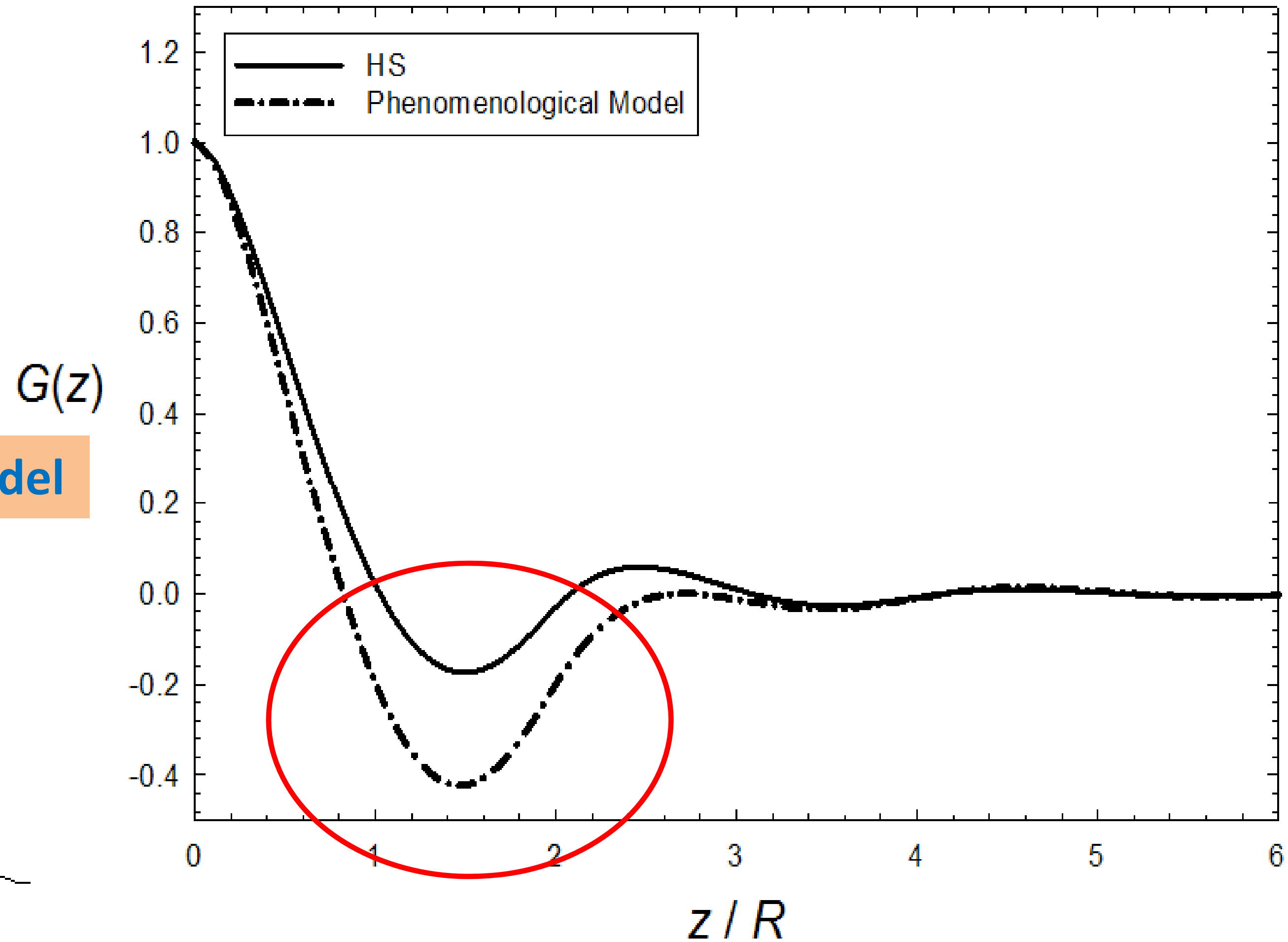

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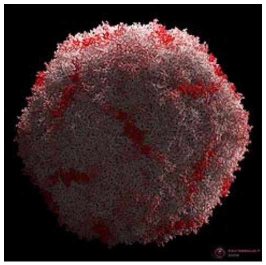
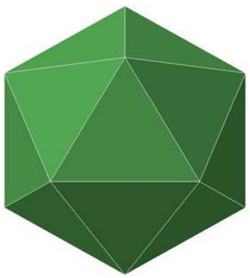
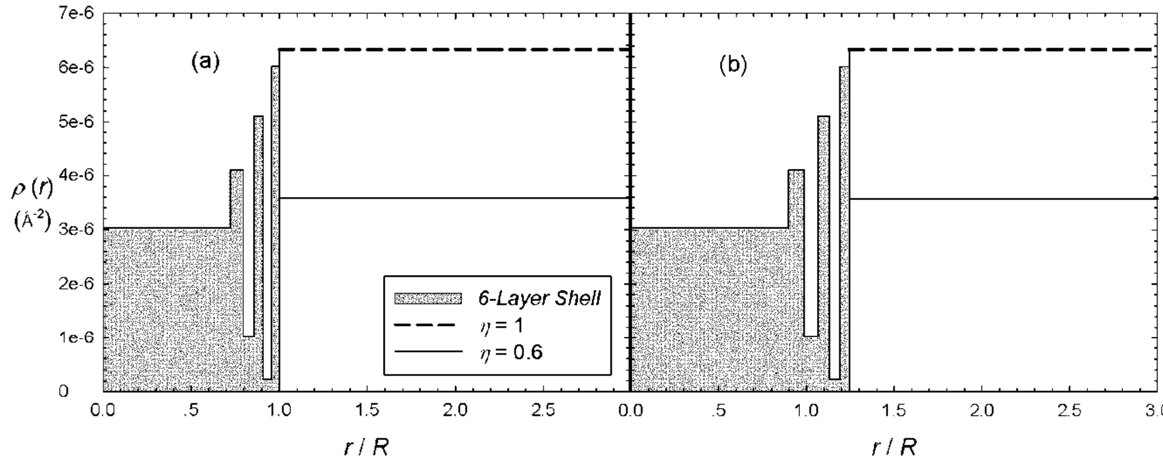
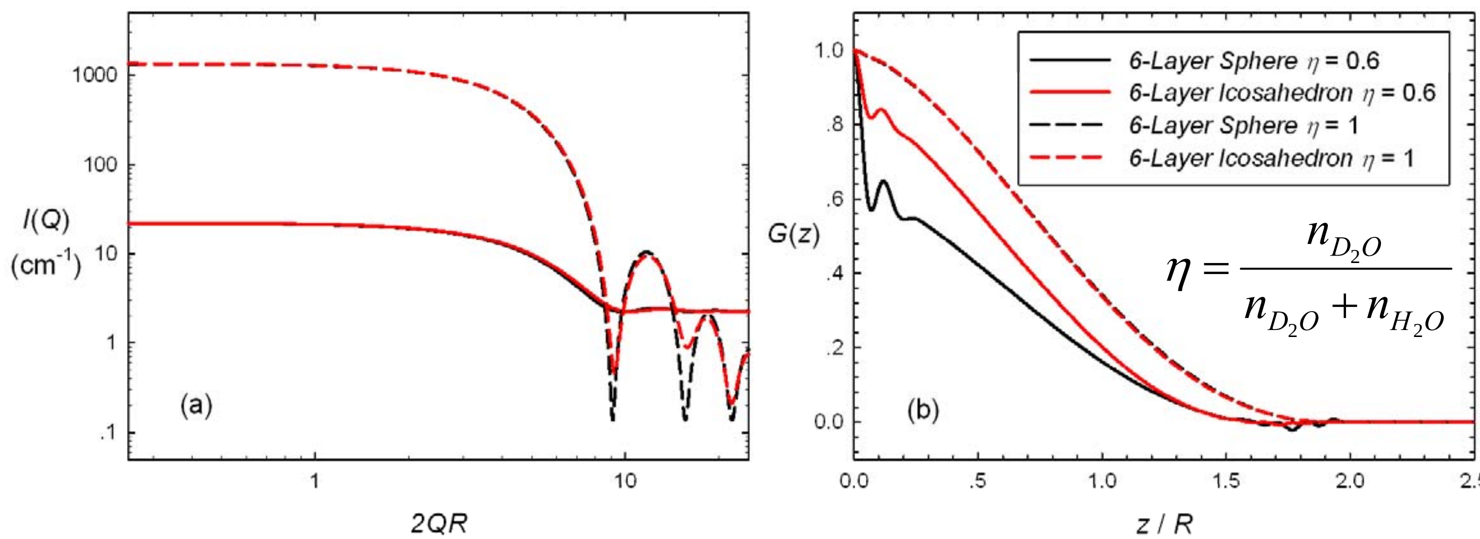
Sensitivity to the geometric shape









Li *et al., J. Phys.: Condens Matter* (submitted)

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Summary

- SESANS length scale: from tens of nm up to several μm

- SESANS correlation function G(z): real space projection

- SESANS advantages:

  direct observation of the spatial distribution

  sensitivity to local structure

  sensitivity to geometric shape

  high concentrated case…

Acknowledgement

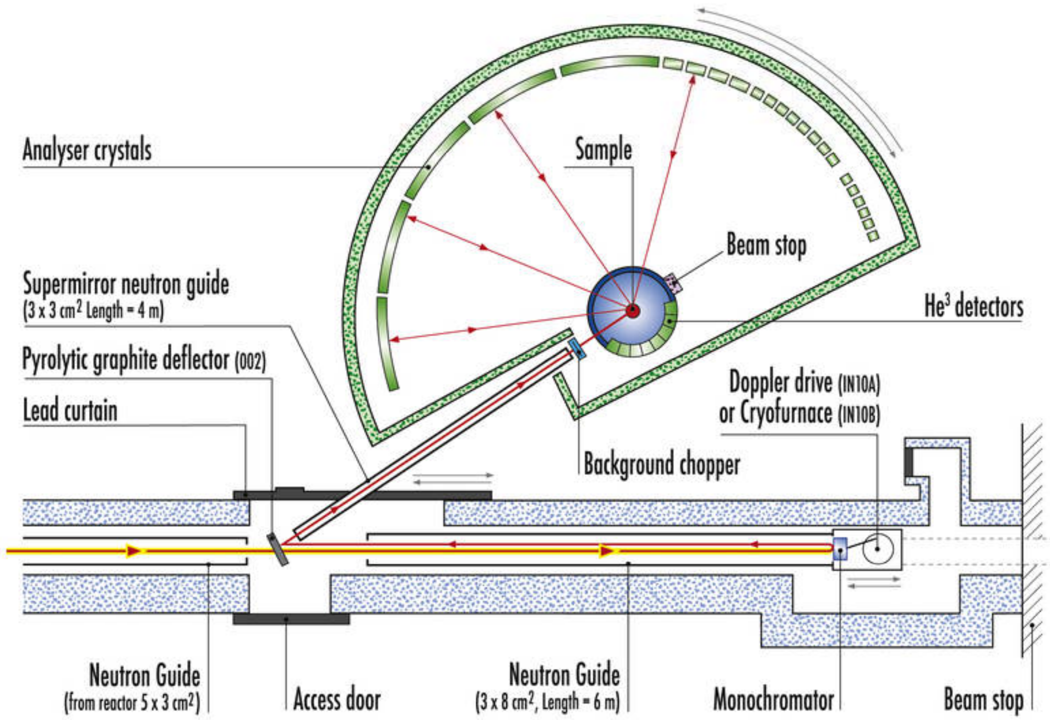
LDRD of ORNL 05272

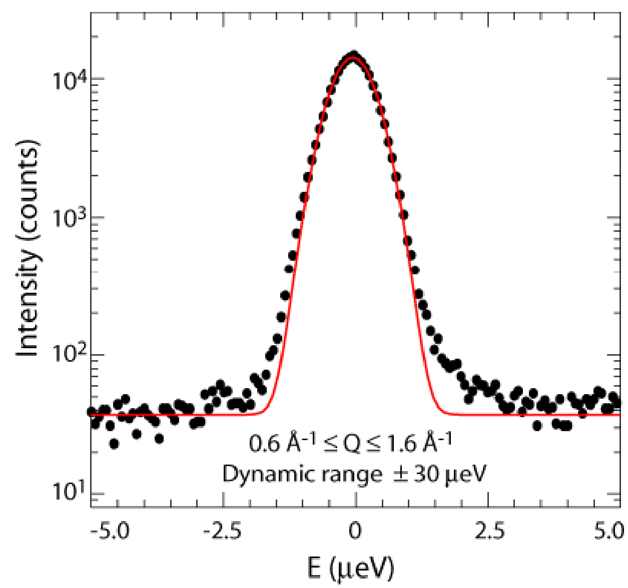
DOE NERI-C Award No. DE-FG07-07ID14889

NRC Award No. NRC-38-08-950

Thank you for your attention!

Backscattering
— measure the dynamics

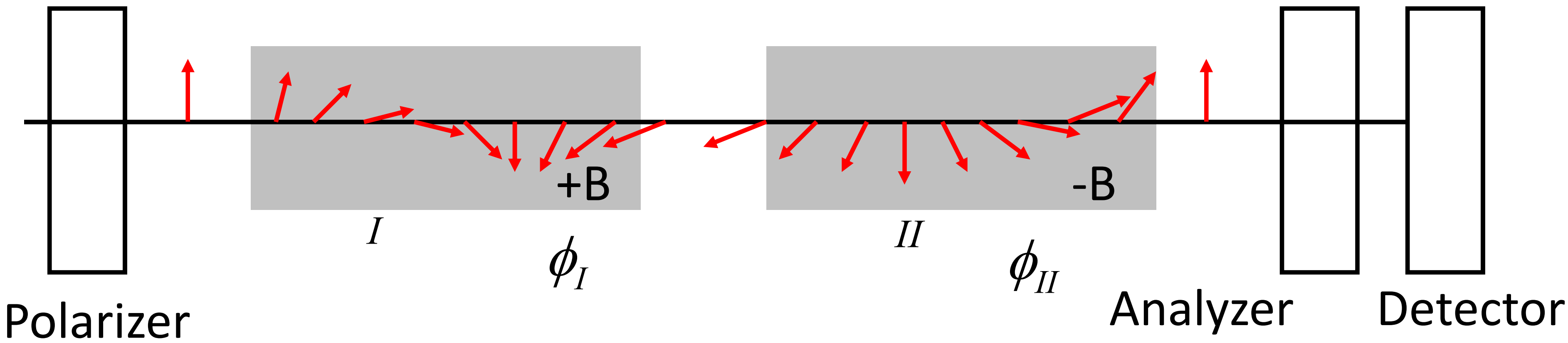




$\hbar\omega = E_i - E_f$

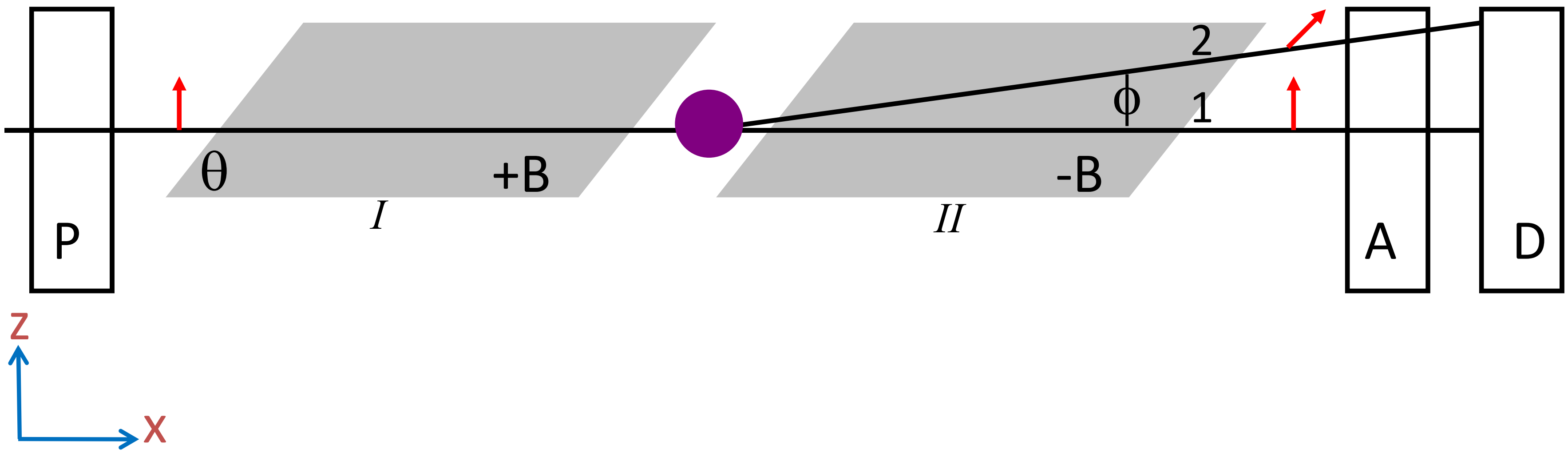
How about probing much slower dynamics (characteristic time > 1 ns)?

Neutron Spin Echo
— measure the dynamics



Mezei, in *Neutron Spin Echo*, Ed. Mezei, Springer 1980

What does SESANS measure?



Pynn, *Lecture 11, Neutron Physics and Scattering*
Indiana University (http://www.iub.edu/~neutron/)

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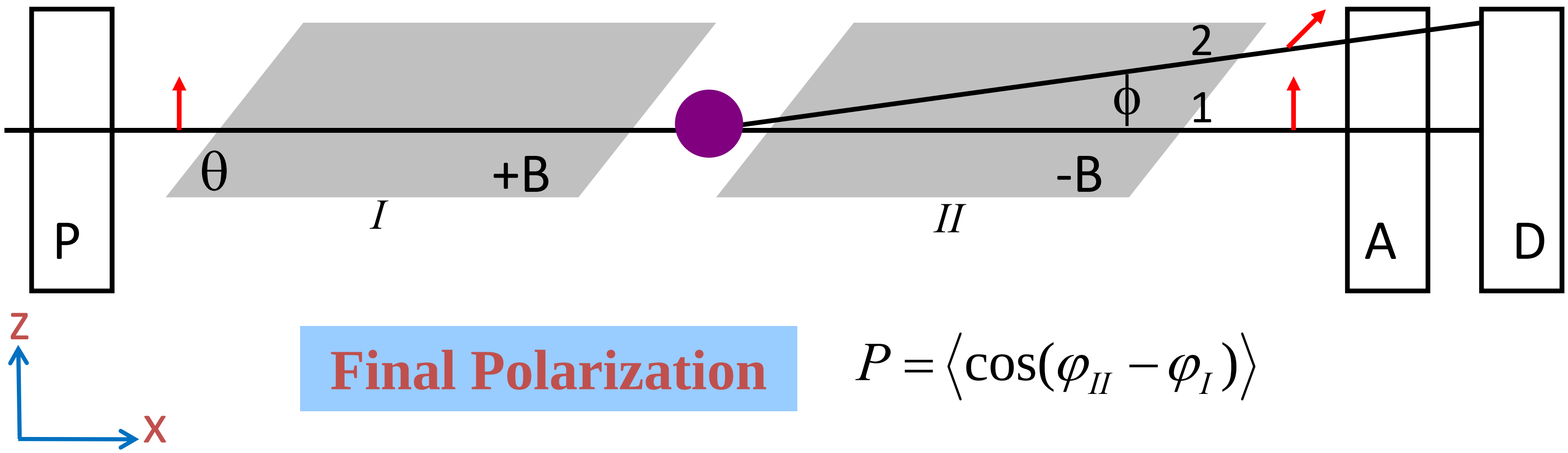
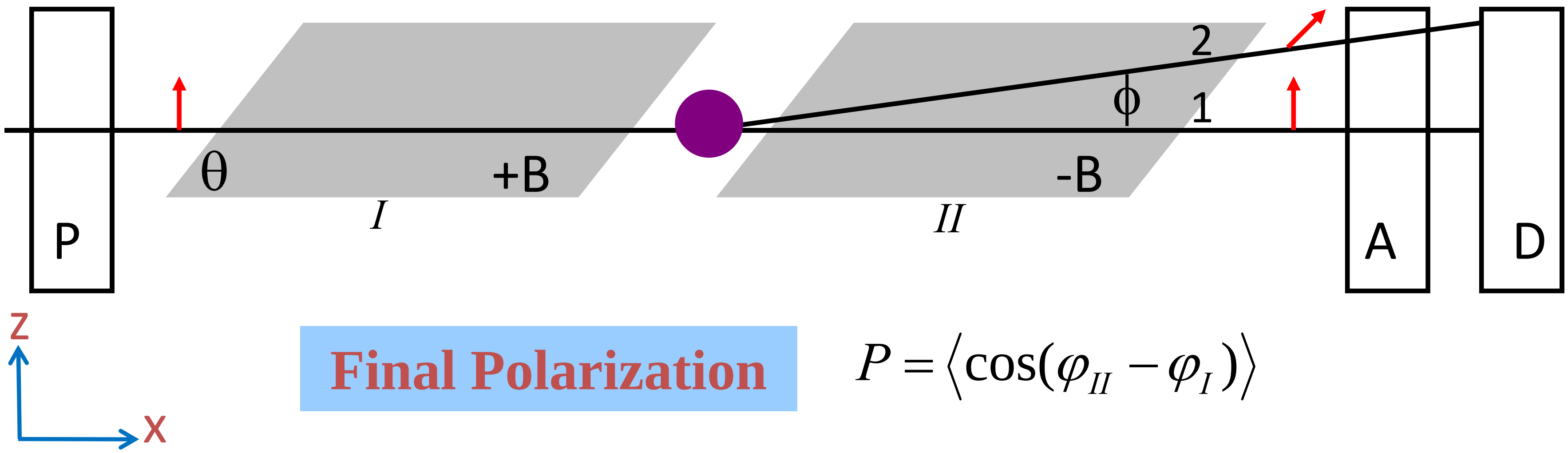


Final Polarization

$$P = \langle \cos(\varphi_{II} - \varphi_{I}) \rangle$$

F. Mezei, Z. Physik, 255 (1972) 145

What does SESANS measure?



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F. Mezei, Z. Physik, 255 (1972) 145

$$\cos(\varphi_{II} - \varphi_I) \approx \cos\left[(cBL\lambda \cot\theta) \cdot \phi\right] = \cos(zQ_z)$$

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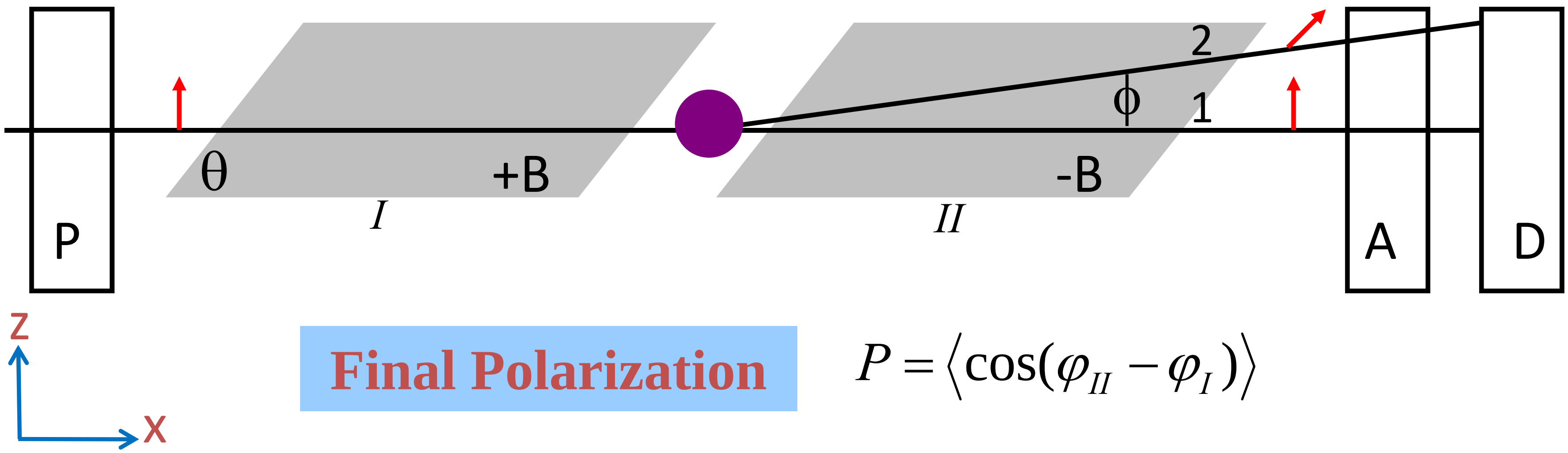
What does SESANS measure?



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F. Mezei, Z. Physik, 255 (1972) 145

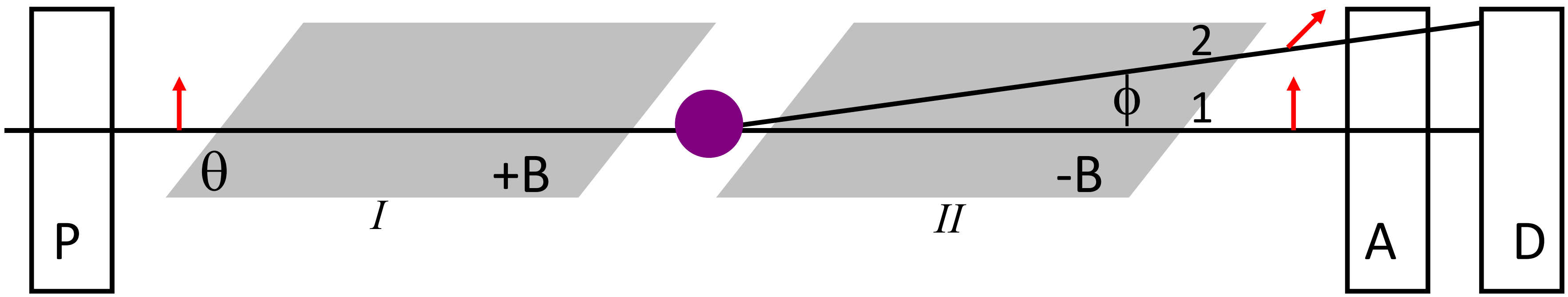
$$\cos(\varphi_{II} - \varphi_I) \approx \cos\left[(cBL\lambda \cot\theta) \cdot \phi\right] = \cos(zQ_z)$$

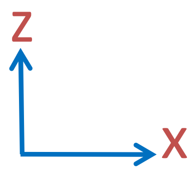
spin-echo length

$$z = \frac{cBL\lambda^2 \cot\theta}{2\pi}$$

Pynn, *Lecture 11, Neutron Physics and Scattering*
Indiana University (http://www.iub.edu/~neutron/)

What does SESANS measure?





Final Polarization $P = \langle \cos(\varphi_{II} - \varphi_I) \rangle$

F. Mezei, Z. Physik, 255 (1972) 145

$$\cos(\varphi_{II} - \varphi_I) \approx \cos[(cBL\lambda \cot\theta) \cdot \phi] = \cos(\underline{\underline{z}} Q_z)$$

spin-echo length

$$z = \frac{cBL\lambda^2 \cot\theta}{2\pi}$$

$$P = \int \frac{d\Sigma}{d\Omega}(\vec{Q}) \cos(\varphi_{II} - \varphi_I) d^3\vec{Q} = \int \frac{d\Sigma}{d\Omega}(\vec{Q}) \cos(zQ_z) d^3\vec{Q}$$

Pynn, *Lecture 11, Neutron Physics and Scattering*
Indiana University (http://www.iub.edu/~neutron/)

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SANS

SESANS

$$I(Q) = \frac{d\Sigma}{d\Omega}(Q)$$

$$G(z) = \int \frac{d\Sigma}{d\Omega}(\vec{Q}) \cos(zQ_z) d^3\vec{Q}$$

O. Spalla, in *Neutron, X-rays and Light: Scattering Methods Applied to Soft Condensed Matter*, edited by P. Linder and Th. Zemb (North-Holland, Amsterdam, 2002), pp. 49–71.

What does SESANS measure?

SANS

SESANS

$$I(Q) = \frac{d\Sigma}{d\Omega}(Q) = \left\langle \int_V \gamma(\vec{r}) \exp(-i\vec{Q}\cdot\vec{r}) d^3\vec{r} \right\rangle$$

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Debye Correlation Function

$$\gamma(\vec{r}) = \frac{1}{V}\int_V \rho(\vec{r}')\rho(\vec{r}'+\vec{r}) d^3\vec{r}'$$

O. Spalla, in *Neutron, X-rays and Light: Scattering Methods Applied to Soft Condensed Matter*, edited by P. Linder and Th. Zemb (North-Holland, Amsterdam, 2002), pp. 49–71.

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Real part of FT in *z* direction

O. Spalla, in *Neutron, X-rays and Light: Scattering Methods Applied to Soft Condensed Matter*, edited by P. Linder and Th. Zemb (North-Holland, Amsterdam, 2002), pp. 49–71.

What does SESANS measure?

SANS

$$I(Q)=\frac{d\Sigma}{d\Omega}(Q)=\left\langle \int_V \underline{\underline{\gamma(\vec{r})}} \exp(-i\vec{Q}\cdot\vec{r})d^3\vec{r} \right\rangle$$

Debye Correlation Function

$$\gamma(\vec{r})=\frac{1}{V}\int_V \rho(\vec{r'})\rho(\vec{r'}+\vec{r})d^3\vec{r'}$$

SESANS

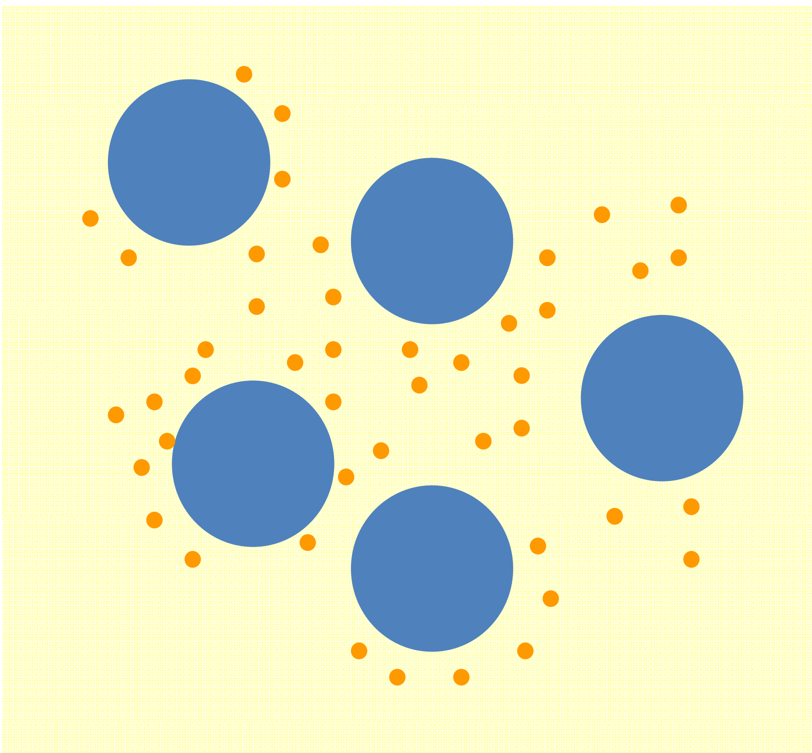
$$G(z)=\int \frac{d\Sigma}{d\Omega}(\vec{Q})\cos(zQ_z)d^3\vec{Q}$$

Real part of FT in *z* direction

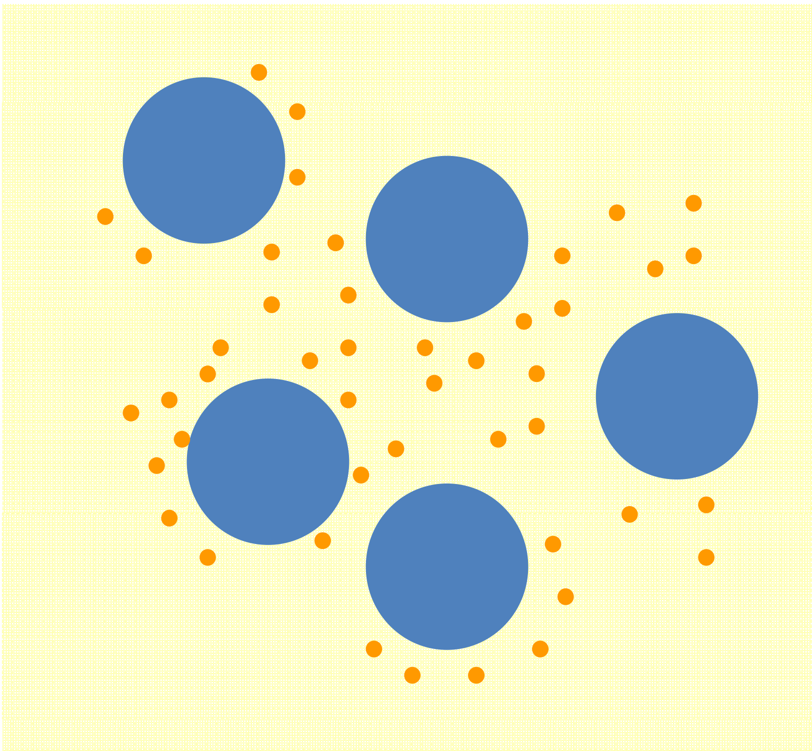
$$G(z)=\int_{-\infty}^{+\infty}\gamma(\vec{r})dx=2\int_z^{+\infty}\frac{\gamma(r)r}{\sqrt{r^2-z^2}}dr$$

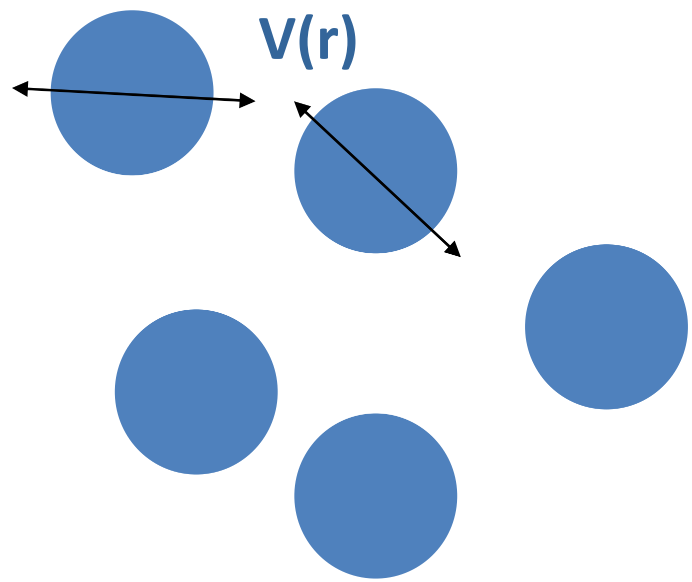
O. Spalla, in *Neutron, X-rays and Light: Scattering Methods Applied to Soft Condensed Matter*, edited by P. Linder and Th. Zemb (North-Holland, Amsterdam, 2002), pp. 49–71.

Real Colloidal System



One Component Model (OCM)

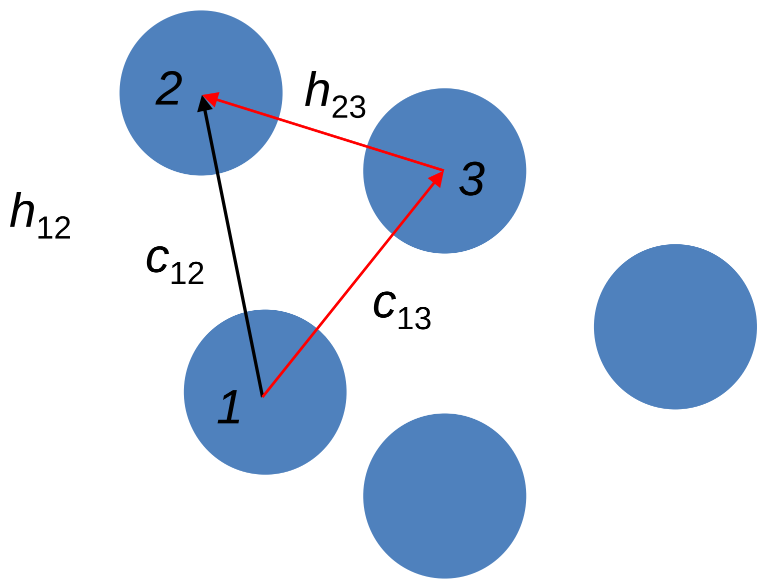


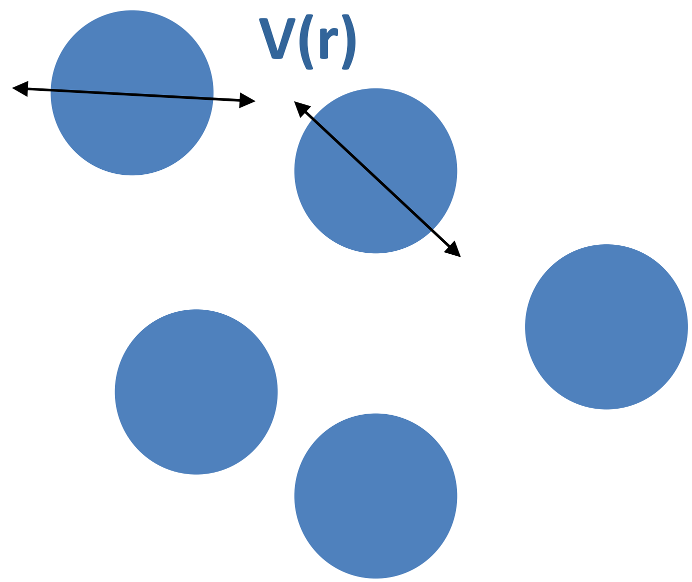


Interaction Potential:

Hard Sphere, Attraction, Repulsion, Ultrasoft potential…

Calculation of Inter-molecular Structure





$$\begin{cases} h(r) = c(r) + n \cdot c(r) \otimes h(r) \\ g(r) = \exp\left[-\beta V(r)\right] \cdot \exp\left[h(r) - c(r) + b(r)\right] \end{cases}$$

Ornstein-Zernike (OZ) equation

Closure equation:
PY, MSA, RY, HNC, ZH…

g*(*r*): the probability to find a particle at a distance of *r

Density Profile **Debye Correlation Function**

$$\rho(\vec{r}) \longrightarrow \gamma(r) = \frac{1}{V}\left\langle \int_V \rho(\vec{r'})\rho(\vec{r'}+\vec{r})d^3\vec{r'} \right\rangle$$

SANS

SESANS

$$I(Q) = \frac{d\Sigma}{d\Omega}(Q) = 4\pi\int_0^\infty \gamma(r)J_0(Qr)r^2 dr$$

Fourier

$$G(z) = 2\int_z^\infty \gamma(r)\frac{r}{\sqrt{r^2-z^2}}dr$$

Abel

Density Profile **Debye Correlation Function**

$$\rho(\vec{r}) \longrightarrow \gamma(r) = \frac{1}{V}\left\langle \int_V \rho(\vec{r'})\rho(\vec{r'}+\vec{r})d^3\vec{r'} \right\rangle$$

SANS

SESANS

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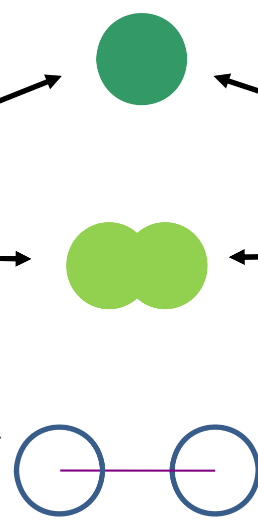
$$G(z) = 2\int_z^\infty \underline{\underline{\gamma(r)}} \frac{r}{\sqrt{r^2 - z^2}} dr$$

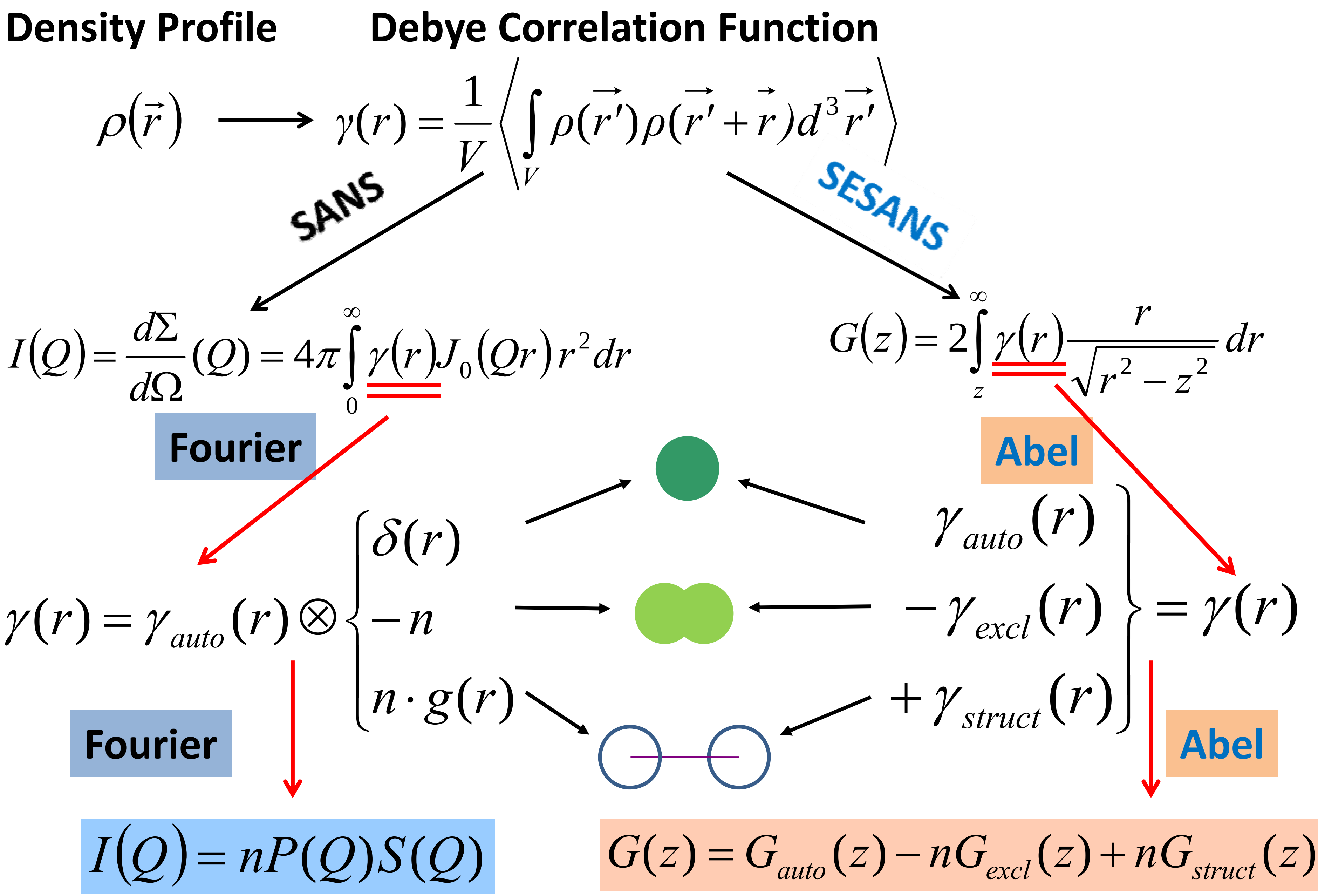
Fourier

Abel



$$\gamma(r) = \gamma_{auto}(r) \otimes \begin{cases} \delta(r) \\ -n \\ n \cdot g(r) \end{cases}$$

$$\left.\begin{matrix} \gamma_{auto}(r) \\ -\gamma_{excl}(r) \\ +\gamma_{struct}(r) \end{matrix}\right\} = \gamma(r)$$



Density Profile
Debye Correlation Function
$\rho(\vec{r}) \longrightarrow \gamma(r) = \frac{1}{V}\left\langle \int_V \rho(\vec{r'})\rho(\vec{r'}+\vec{r})d^3\vec{r'} \right\rangle$
SANS
SESANS
$I(Q) = \frac{d\Sigma}{d\Omega}(Q) = 4\pi\int_0^\infty \gamma(r)J_0(Qr)r^2dr$
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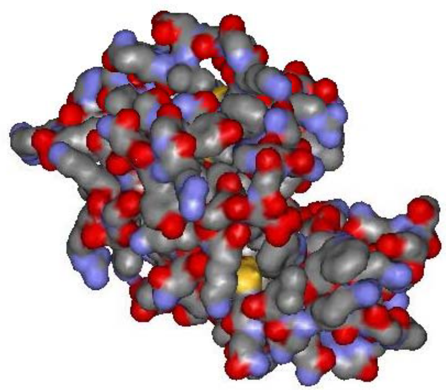
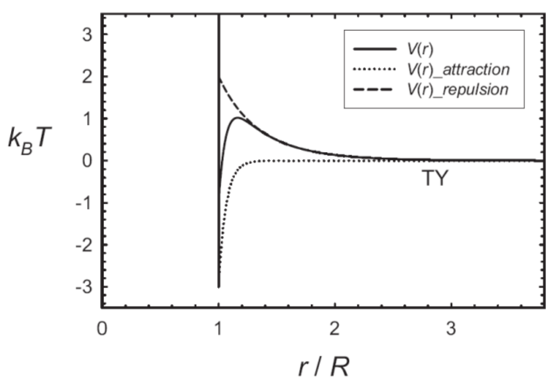
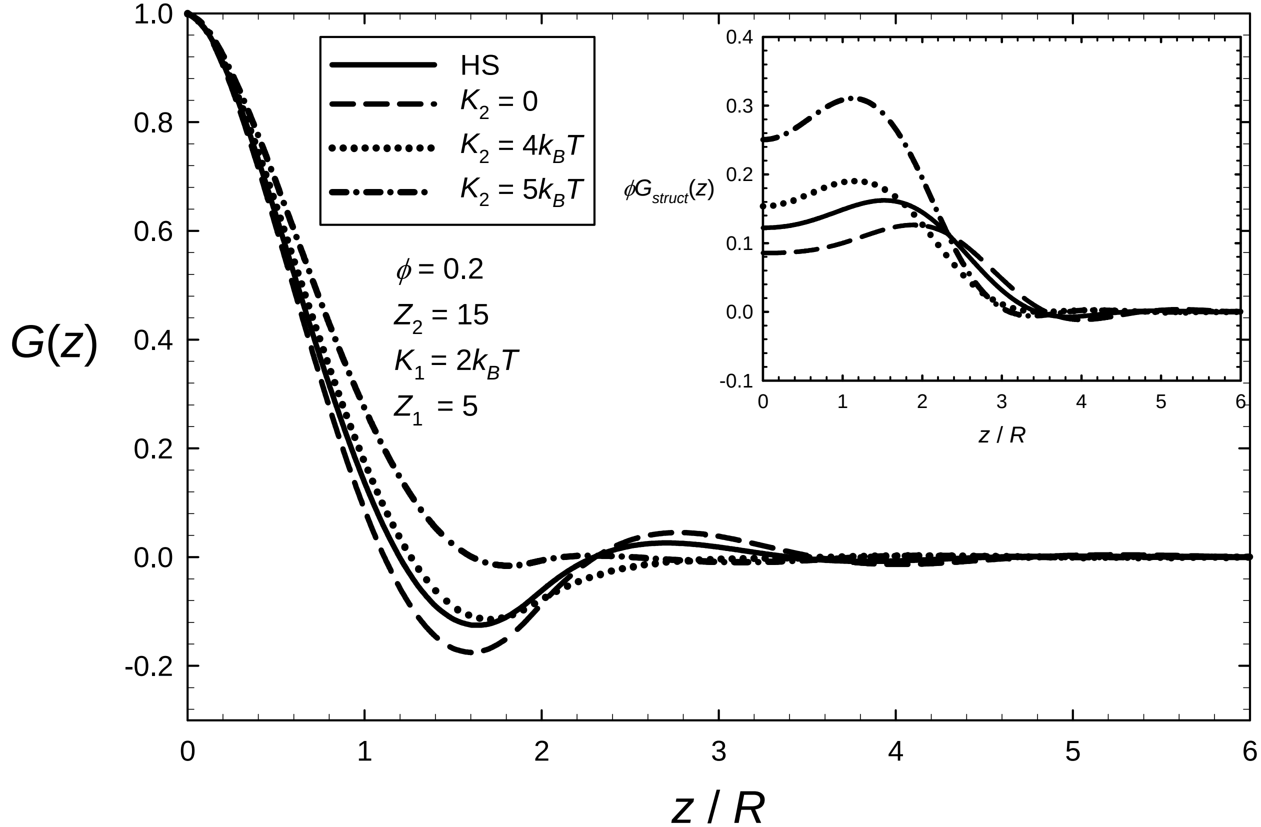
Fourier
Abel
$\gamma(r) = \gamma_{auto}(r) \otimes \begin{cases} \delta(r) \\ -n \\ n \cdot g(r) \end{cases}$
$\left.\begin{matrix} \gamma_{auto}(r) \\ -\gamma_{excl}(r) \\ +\gamma_{struct}(r) \end{matrix}\right\} = \gamma(r)$
Fourier
Abel
$I(Q) = nP(Q)S(Q)$
$G(z) = G_{auto}(z) - nG_{excl}(z) + nG_{struct}(z)$

Example IV: Two-Yukawa Potential



$$V(r)=\begin{cases}\infty & r<R\\ K_1\dfrac{\exp[-Z_1(r-2R)]}{r}-K_2\dfrac{\exp[-Z_2(r-2R)]}{r} & r>R\end{cases}$$

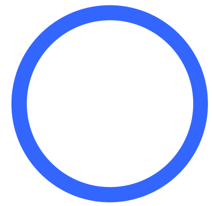




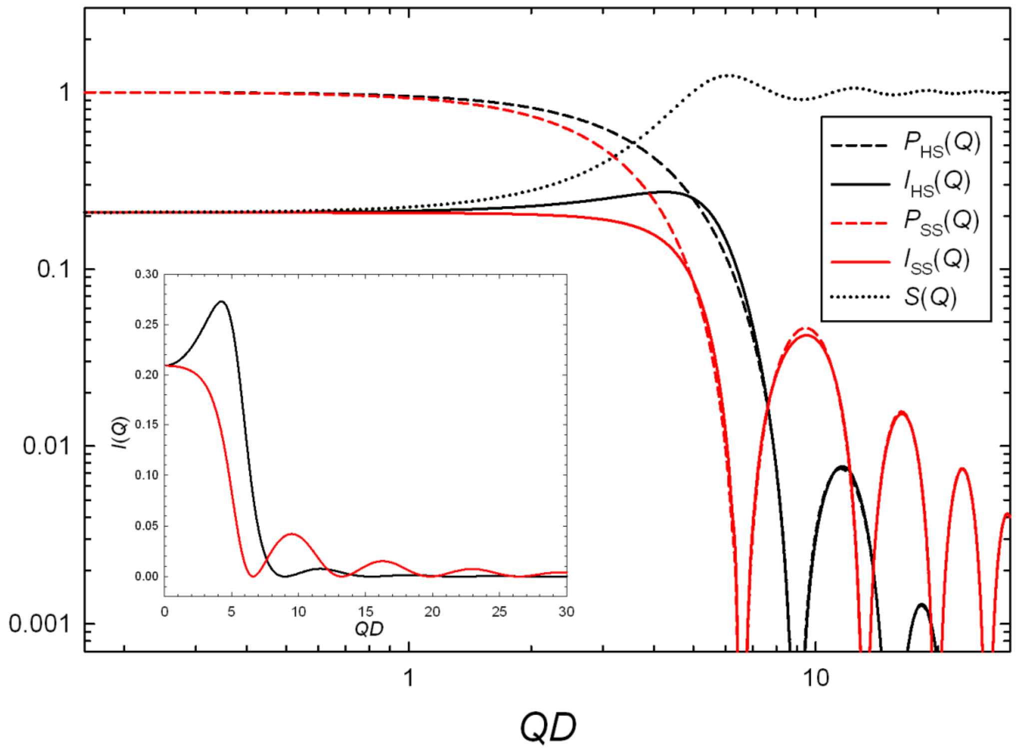
Li *et al., J. Chem. Phys.* **132** 174509 2010

Sensitivity to radial density profile: spherical core-shell

homogeneous
hard sphere

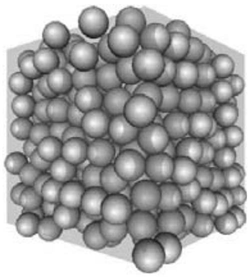


spherical
shell

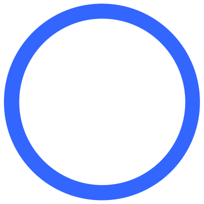


Li *et al., J. Chem. Phys.* **134** 094504 2011

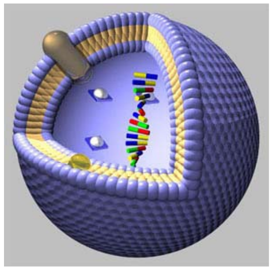
Sensitivity to radial density profile: spherical core-shell

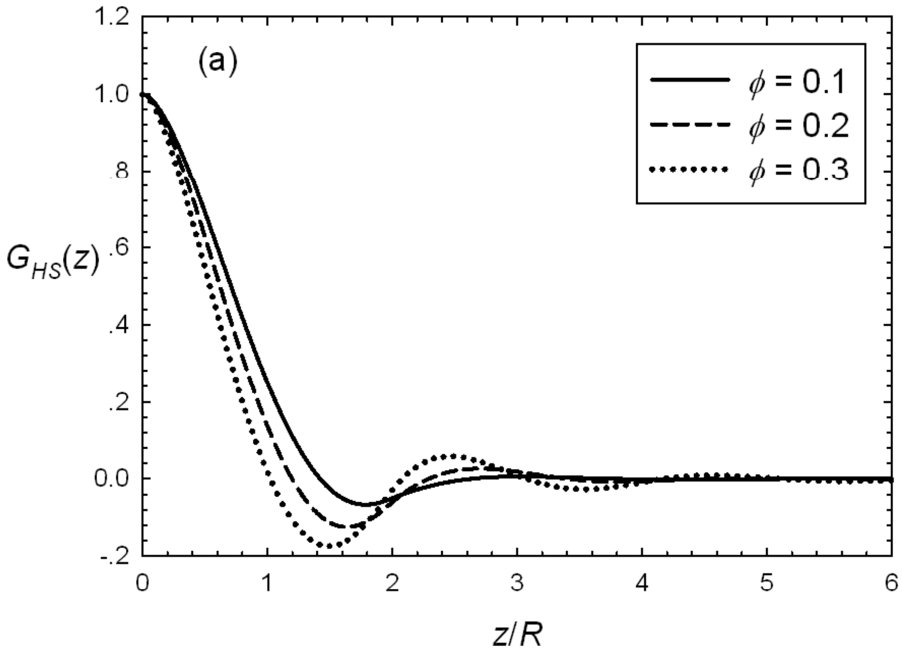


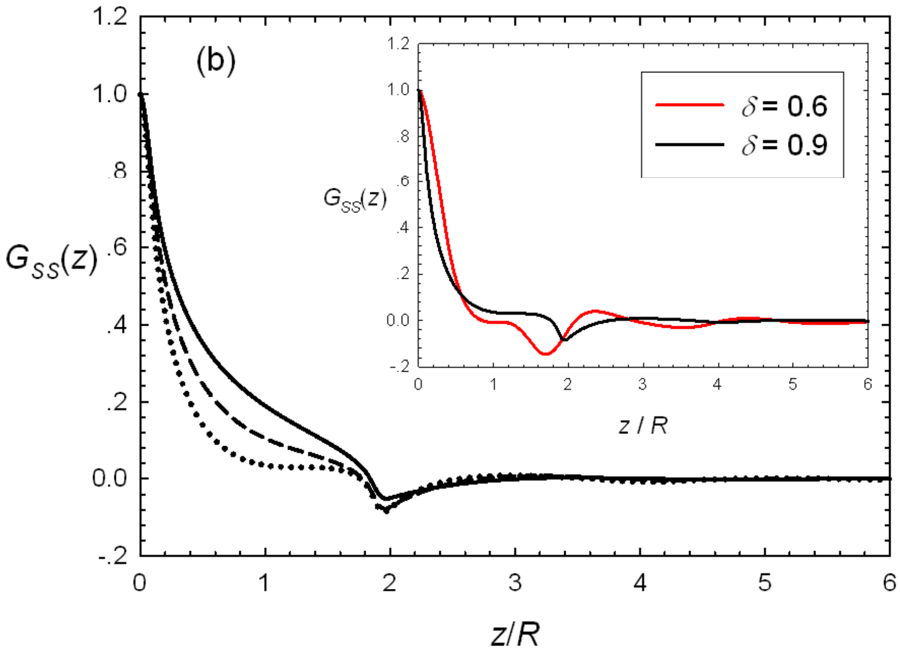
homogeneous
hard sphere



spherical
shell

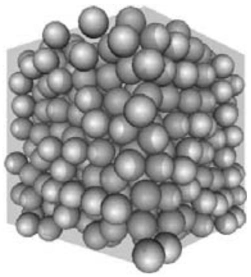






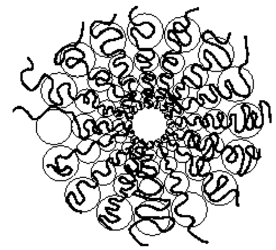
Li *et al., J. Chem. Phys.* **134** 094504 2011

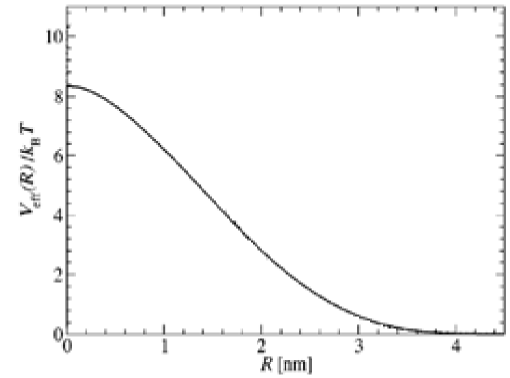
Soft colloid



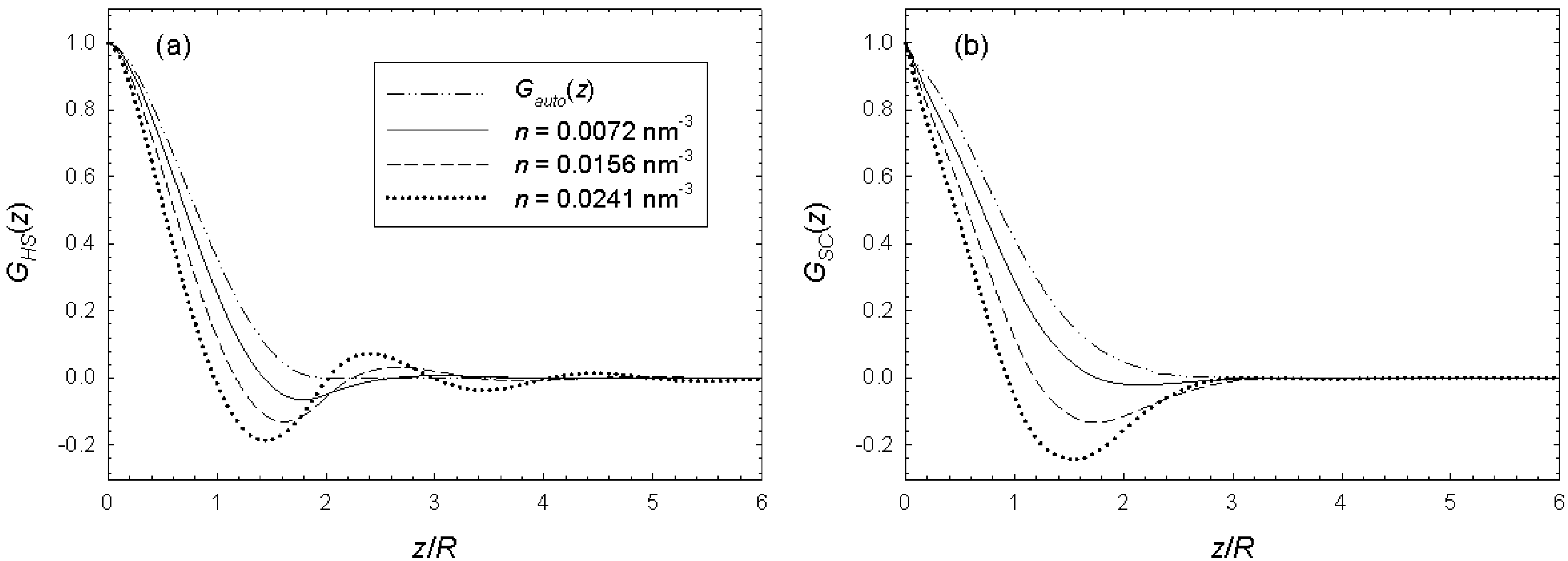
homogeneous hard sphere

soft colloid



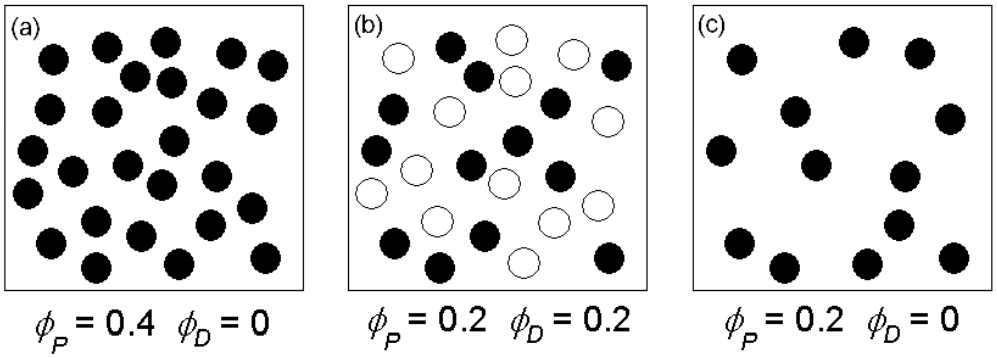


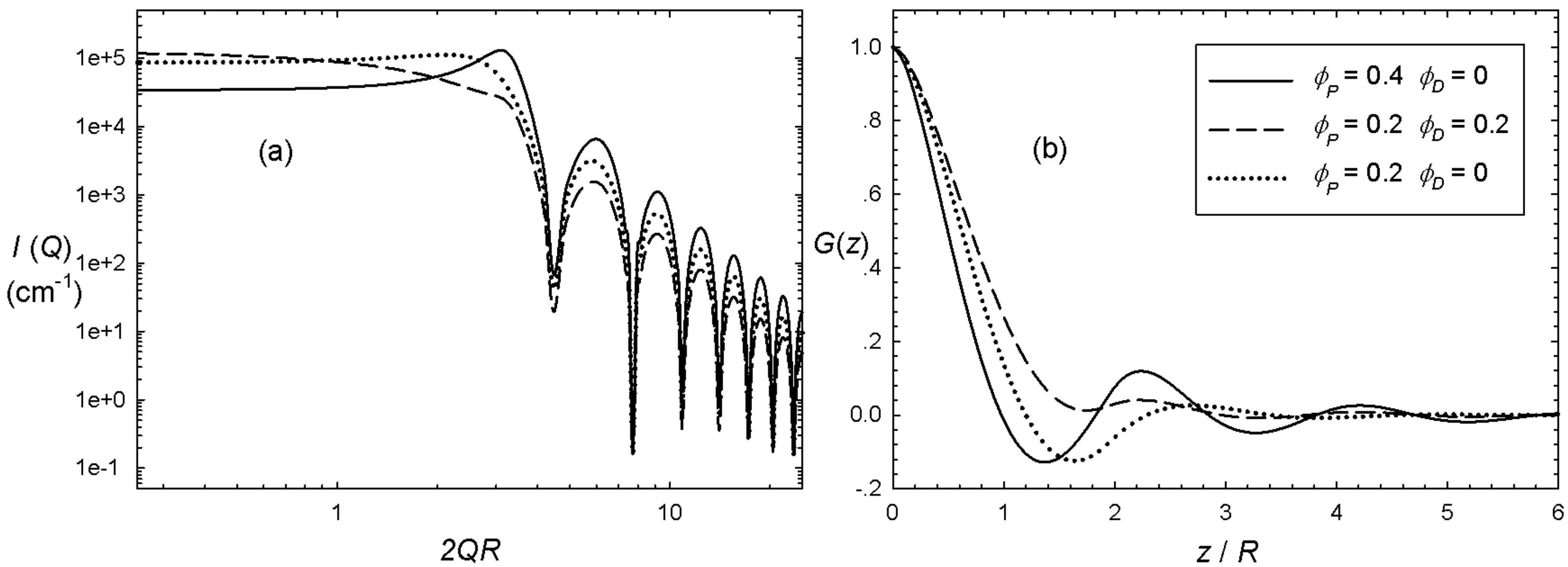
***n*=0.0379 nm^{-3}**



Li *et al., J. Chem. Phys.* **134** 094504 2011

Create a contrast: D/H mixture

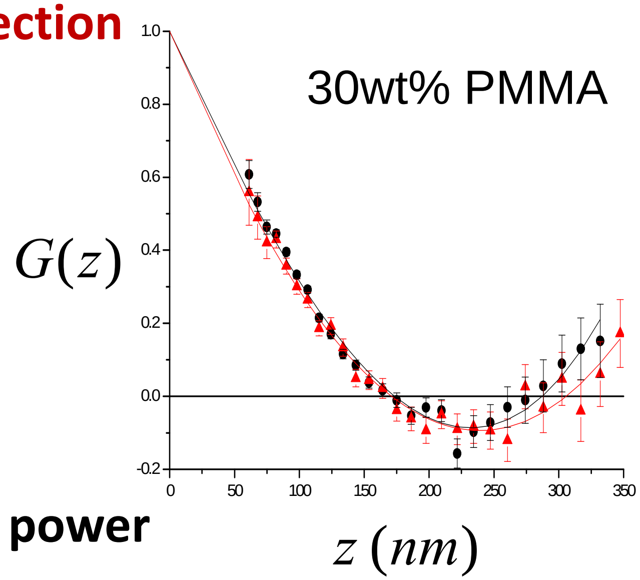




Li *et al., J. Phys.: Condens Matter* (submitted)

Summary

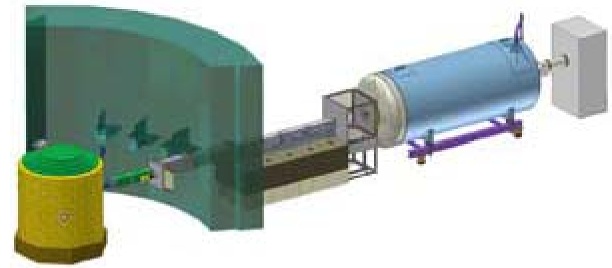
- SESANS length scale: from tens of nm up to several μm
- SESANS correlation function G(z): real space projection
- SESANS advantages:
  - sensitivity to local structure
  - sensitivity to structural heterogeneity
  - high concentrated case…
- SESANS disadvantage: no sensitivity to scattering power



SESANS spectrometers

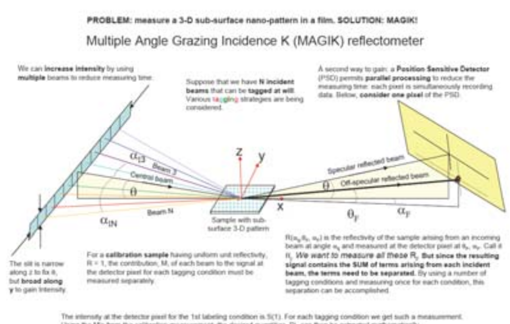
Delft University Nederland (2002)

Asterix at LANSCE LANL US (2009)

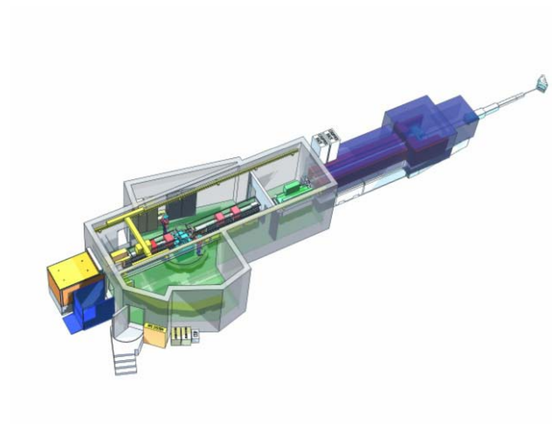


SESAME at LENS IU US (2010)

OFFSPEC at ISIS UK (2010)



MAGIK at NCNR NIST US (2013)



Larmor at ISIS UK (2014)

Multiple Scattering

$$P(z) = T + G'(z,t)$$

$$\rho_n = \frac{t^n \int dQ_{1y} dQ_{1z} \frac{d\sigma}{d\Omega}(Q_1)}{k_0^{2n} 1 \times 2 \times \cdots \times n}$$

$$\times \int dQ_{2y} dQ_{2z} \frac{d\sigma}{d\Omega}(Q_2) \cdots \int dQ_{ny} dQ_{nz} \frac{d\sigma}{d\Omega}(Q_n) \times T$$

$$= \frac{(\sigma t)^n}{n!} T$$

$$Q_1 + Q_2 + \cdots Q_n = Q$$

$$T = \exp(-\sigma t)$$

$$\cos(Q_z) = \cos(Q_{1z})\cos(Q_{2z}) \cdots \cos(Q_{nz}) + odd\ terms$$

Multiple Scattering (Continue…)

$$\rho_n' = \frac{t^n \int dQ_{1y} dQ_{1z} \frac{d\sigma}{d\Omega}(Q_1)\cos(Q_{1z}z)}{k_0^{2n} 1\times 2\times\cdots\times n} \times \int dQ_{2y} dQ_{2z} \frac{d\sigma}{d\Omega}(Q_2)\cos(Q_{1z}z)$$

$$\times\cdots\int dQ_{ny} dQ_{nz} \frac{d\sigma}{d\Omega}(Q_n)\cos(Q_{1z}z)\times T = \frac{\left(\sigma G(z)t\right)^n}{n!} T$$

$$G'(z,t) = \sum_n \rho_n' = \sum_{n=1} \frac{(\sigma G(z)t)^n}{n!} T = T(e^{\sigma G(z)t} - 1)$$

$$G(z) = 1 - \frac{\ln(P(z))}{\ln(T)},\ P(z) = e^{\sigma t(G(z)-1)}$$

$$G(\infty) = 0,\ P(\infty) = T = e^{-\sigma t}$$

$$G(0) = 1,\ P(0) = 1$$

Dynamic vs. Structural

$$\varphi_I = \frac{\omega L}{v}$$

$$\varphi_{II} = \frac{\omega L}{(v+\Delta v)\sin(\theta+\alpha)} \approx \frac{\omega L}{(v+\Delta v)(1+\alpha\cot\theta)}$$

$$\Delta\varphi = \varphi_{II} - \varphi_I = \frac{\Delta v + \alpha v\cot\theta + \alpha\Delta v\cot\theta}{v(v+\Delta v)(1+\alpha\cot\theta)}\omega L \approx \frac{\Delta v}{v^2}\omega L + \frac{\alpha\cot\theta}{v}\omega L$$

The ratio:

$$\frac{dynamic}{structural} = \frac{\Delta v / v}{\alpha\cot\theta} = \frac{\Delta E / E}{2\alpha\cot\theta}$$

$$\Delta E \sim \mu eV,\; E \sim meV$$

$$\alpha \sim 1^o,\; \theta = 20^o$$

Stokes-Einstein equation: $D_0 = \dfrac{k_B T}{6\pi\eta R}$