Spin Echo Small-Angle Neutron Scattering

SESANS - 101

Introductory Concepts

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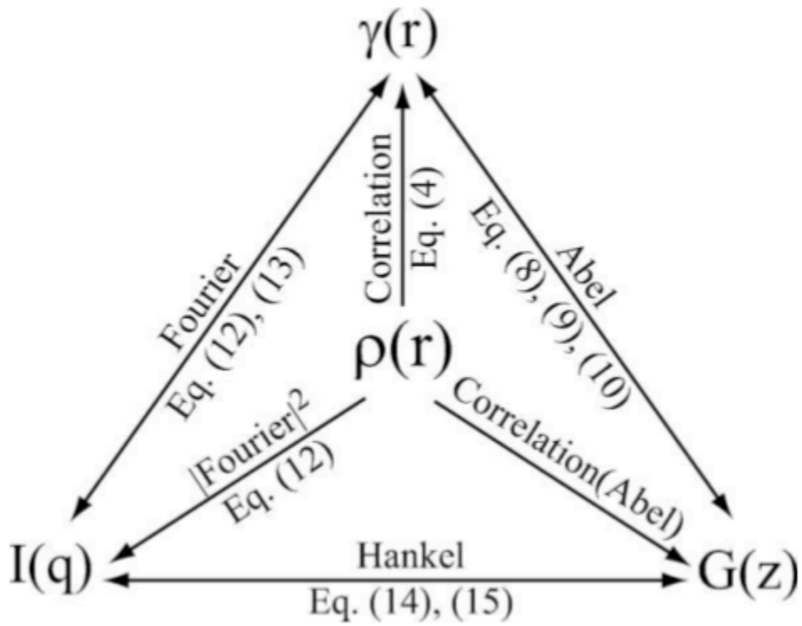
Real Space Information…

STANDARD SANS



SESANS

Figure 1
The relationship between the Abel, Hankel and Fourier transformations for an isotropic distribution $\rho(r)$. Note that $G(z)$ can be found by calculating the autocorrelation function of the projection of $\rho(r)$.

Andersson et al *J. Appl. Cryst.* (2008). **41**, 868–885

Fourier Transform

$$\gamma(r) = \frac{1}{2\pi^2} \int_0^\infty \frac{\sin(qr)}{qr} I(q)\, q^2\, \mathrm{d}q. \tag{13}$$

Hankel Transform

$$G(z) = (2\pi\xi)^{-1} \int_0^\infty J_0(qz)\, I(q)\, q\, \mathrm{d}q, \tag{14}$$

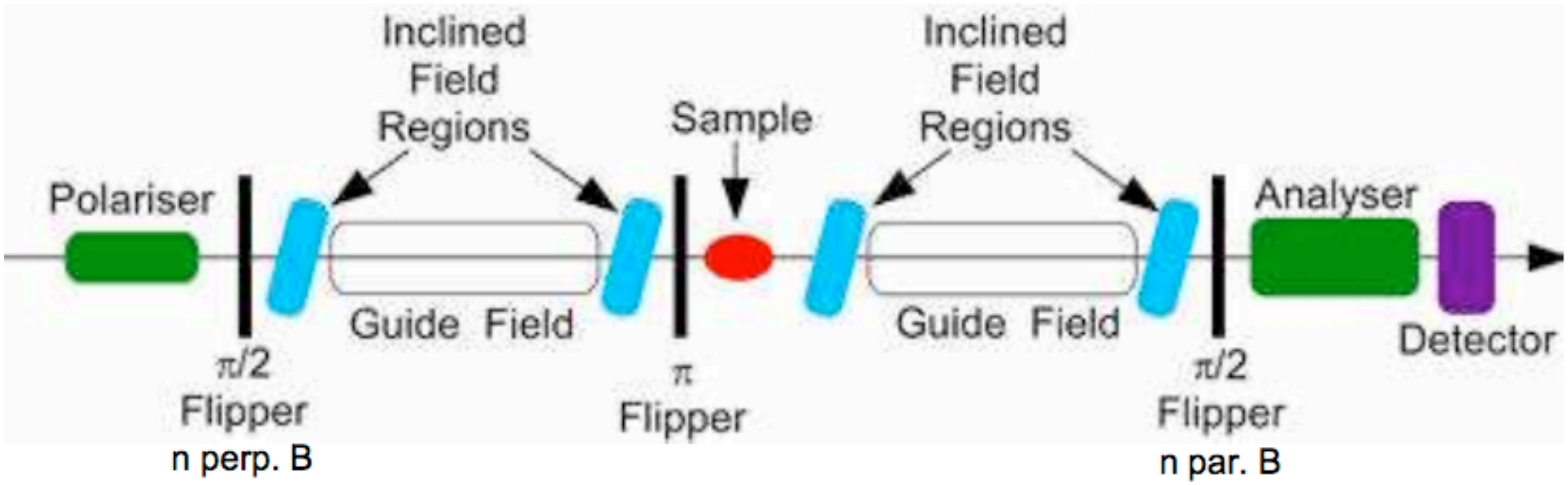
Abel Transforms

For a spherically symmetric (*i.e.* isotropic) density distribution the projection $G(z)$ can be written as

$$G(z) = \frac{2}{\xi} \int_z^\infty \frac{\gamma(r) r}{(r^2 - z^2)^{1/2}}\, \mathrm{d}r. \tag{8}$$

Provided that $\gamma(r)$ decays to zero faster than $1/r$, the inverse transformation is found as

$$\gamma(r) = -\frac{\xi}{\pi} \int_r^\infty \frac{G'(z)}{(z^2 - r^2)^{1/2}}\, \mathrm{d}z, \tag{9}$$



Dedicated SESANS Instrument since ~1999
Delft, Netherlands

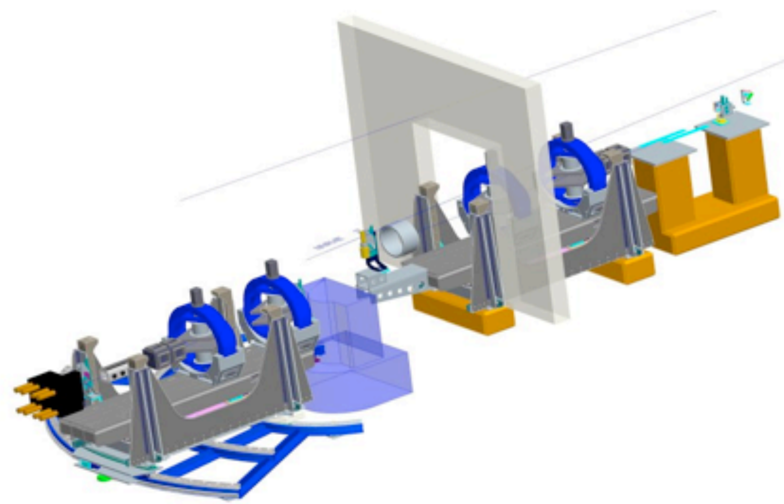
Offspec: spin-echo reflectometer

{ Partnered with Delft group }

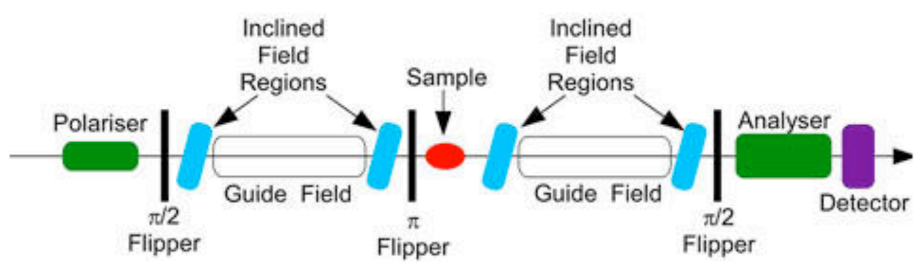
An increasing number of important science and technology issues in the study of interfaces, thin films and multilayers depend on knowledge of the structure in the plane of the interface.

Demand for techniques to understand such structures is growing substantially in relation to spin electronics, plastic electronics, patterned sub-phases, membranes, proteins, dewetting polymers, surfactant systems, lubricants, coatings and sensors.

Offspec is an advanced reflectometer giving access to nanometre length scales parallel and perpendicular to interfaces, using the technique of spin-echo to decode the path neutrons have take through the instrument. By enabling the explicit separation of specular and off-specular reflectivity, new surface structures such as patterned data storage media, mesoporous films and biological membranes can be probed.



The length scale coverage of Offspec will be comparable to those studied by atomic force microscopy, scanning tunnel microscopy and other more invasive surface profiling techniques.



Delft instrument:

Beam current: 900 s^{-1}

Divergence: 0.006 Rad (vert+Horz)

Wavelength: λ = 2.1 Å, $\Delta\lambda/\lambda$ = 1 %

Instrument length: 7 m

Move to Cold guide at NCNR:

Change wavelength: λ = 4.75 Å, $\Delta\lambda/\lambda$ = 1 %

Increase z by factor $(\lambda_{new}/\lambda_{old})^2 = 5$

Assume loss from Guide, polarizers, air $T_L = 0.1$

Beam current: 44,000 s^{-1}

{ Comparable to BT5 USANS !!! }

Extracted from C. Rehm ANSTO draft report

2.1 Instrument Components and Operating Mode

The SESANS experiment detects changes in neutron polarization after neutrons have passed through two equal and opposite Larmor precession fields located before (red diamond) and after the sample (blue diamond). A schematic presentation of the experimental set-up is shown in Fig. 6.

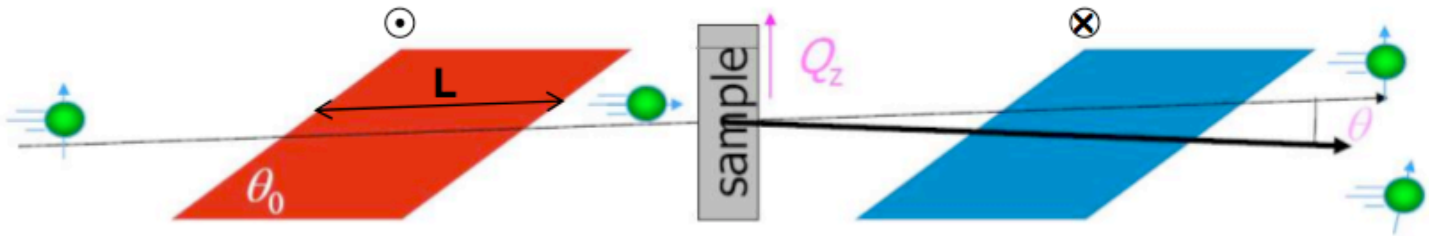


Figure 6
Schematic SESANS arrangement [10]

In the absence of the scattering sample, the neutron polarization vector will precess in opposite directions by an equal amount within each of the two precession fields. At the exit of the second Larmor device, the net precession becomes zero, and the neutron polarization vector is restored to its original state from before the precession had started.

In the presence of a scattering sample, the scattered neutrons will have different path lengths within the second Larmor device. The opposing precessions of these scattered neutrons within the two Larmor fields will no longer cancel each other. The final polarization of these scattered neutrons will be lower from that of the transmitted ones. Thus, the neutron scattering angles are encoded into the neutron polarization. The detection of the final neutron polarization at the analyzer yields a real space correlation function of the sample, namely the spin-echo length z (= distance between two scattering volumes in the sample) with

$$z = \frac{c \cdot \lambda^2 \cdot B \cdot L \cdot \cot \theta_0}{2 \cdot \pi} \qquad (1)$$

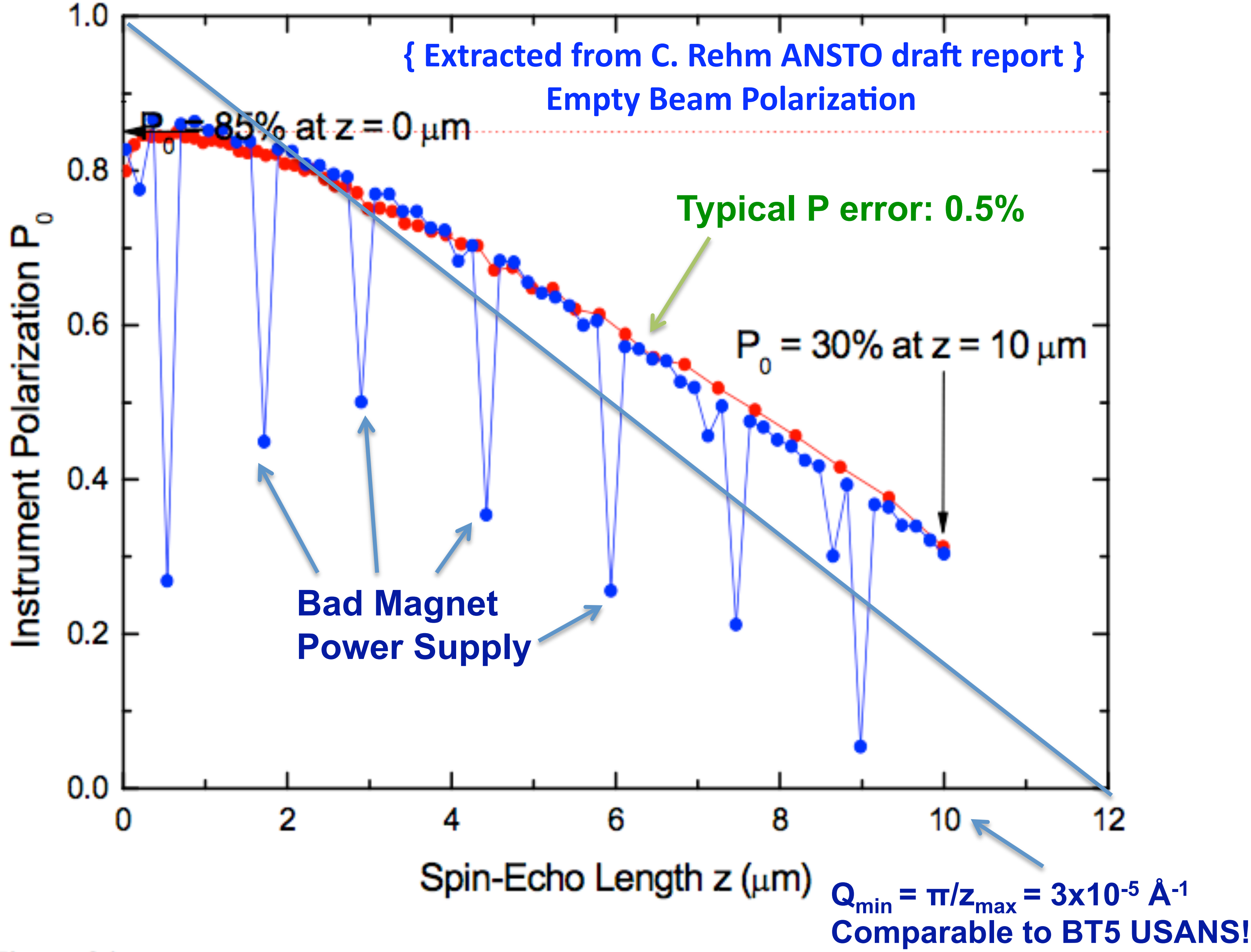


Figure 24
Delft SESANS instrument polarization decreases with increasing spin-echo length z

$$P(z) = \exp\{\Sigma_t[G(z) - 1]\}, \quad (20)$$

τ

$G(z) = 1 + \ln(P_s/P_0) / \tau$

$P = (N^+ - N^-) / (N^+ + N^-)$

$\sigma_P^2 = 1 / N_T$ where $N_T = N^+ + N^-$

For $\tau \approx 0$, { single scattering limit…. }

$\ln(P_s/P_0) \cong -1 + P_s/P_0$

$G(z) \cong 1 - 1/\tau + P_s/(\tau P_0)$

$\sigma_G^2 \cong (P_0^2 + P_S^2) / (\tau^2 N_T P_0^4)$

Since $P_S \cong P_0$

$\boldsymbol{\sigma_G \cong (2/N_T)^{1/2} / (\tau P_0)}$

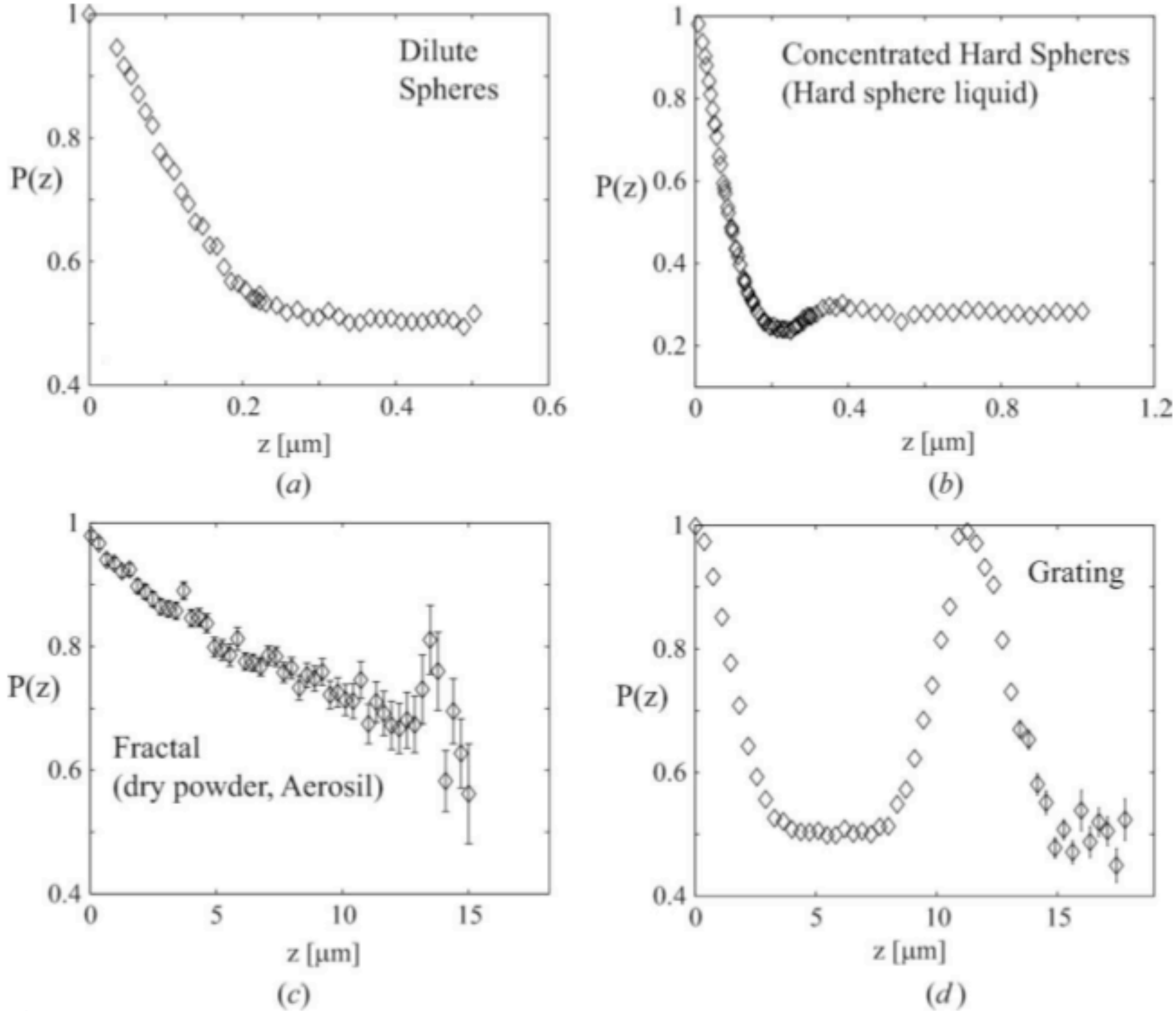


Figure 3
SESANS measurements conducted on various samples. (*a*) A measurement on a dilute sample of sterically stabilized silica spheres. (*b*) The result from a more concentrated dispersion of silica spheres. For more information on measurements (*a*) and (*b*) see Krouglov, Bouwman *et al.* (2003). (*c*) A measurement on a dry nano-powder of silica. (*d*) A measurement of a grating made up of periodic silicon beams.

5.2. Random two-phase media

For a perfectly random inhomogeneous solid, Debye, Anderson and Bueche (DAB; Debye *et al.*, 1957; Debye & Bueche, 1949) conjectured that

$$\gamma(r) = \exp(-r/a), \tag{52}$$

where a represents a measure of the size of the random inhomogeneities. The argument for the validity of this relation is that its series expansion at small r yields equation (37). The projection of this correlation function is

$$G(z) = (z/a)\, K_1(z/a), \tag{53}$$

where K_n is the modified Bessel function of the second kind. The Fourier power spectrum is

$$I(q) = \frac{8a^3\pi}{\left[1 + (qa)^2\right]^2}. \tag{54}$$

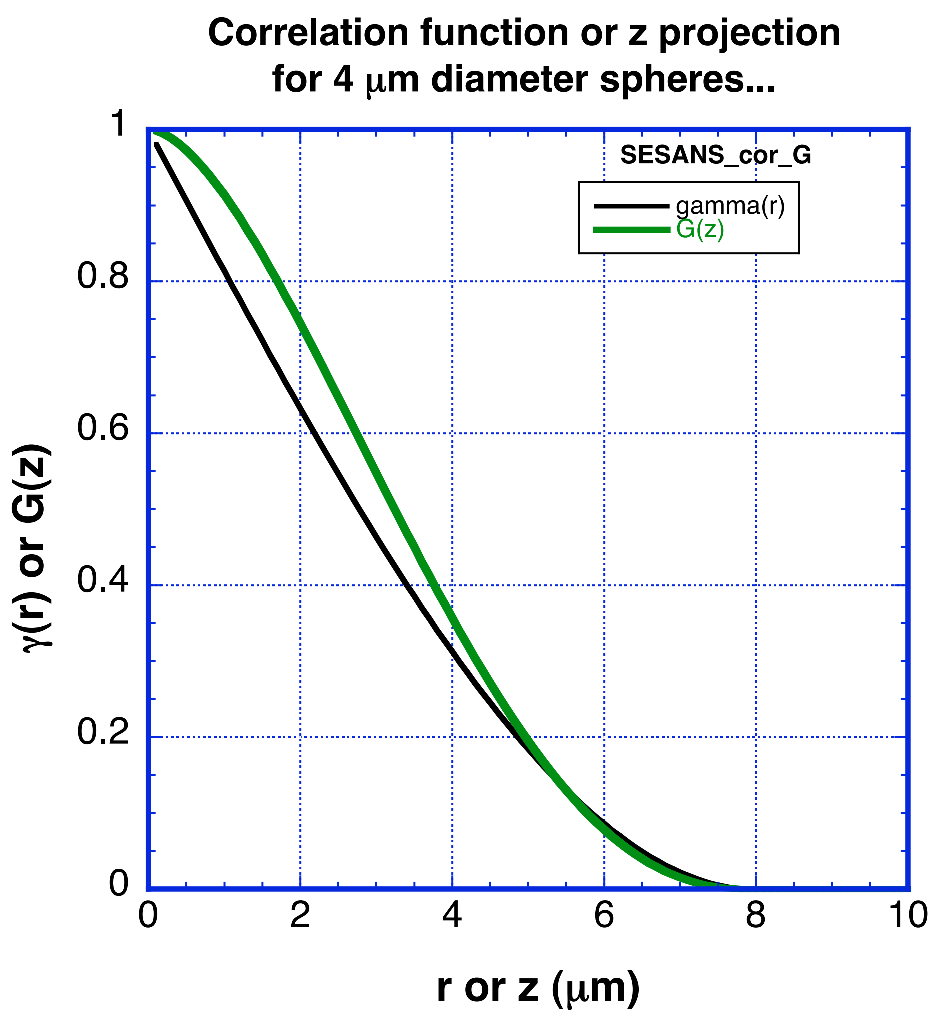
6.1. Sphere

For a single sphere with radius R the autocorrelation function is

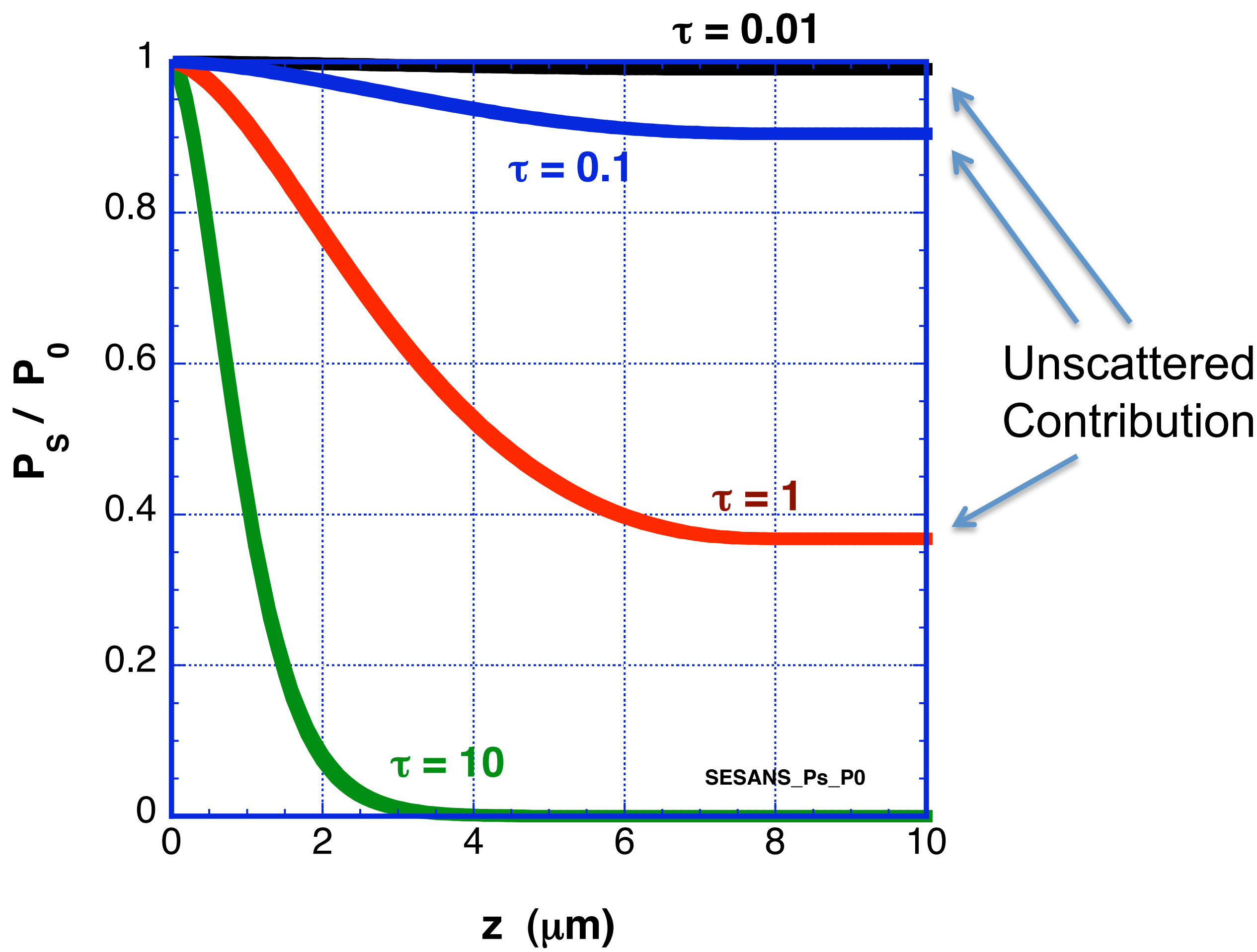
$$\gamma(r) = 1 - \frac{3}{4}\frac{r}{R} + \frac{1}{16}\left(\frac{r}{R}\right)^3 \tag{60}$$

for $r \leq 2R$ and zero elsewhere. The corresponding projection $G(z)$ is found by inserting equation (60) into equation (8) and integrating from zero to $2R$; this gives for $z \geq 0$ (Krouglov, de Schepper *et al.*, 2003)

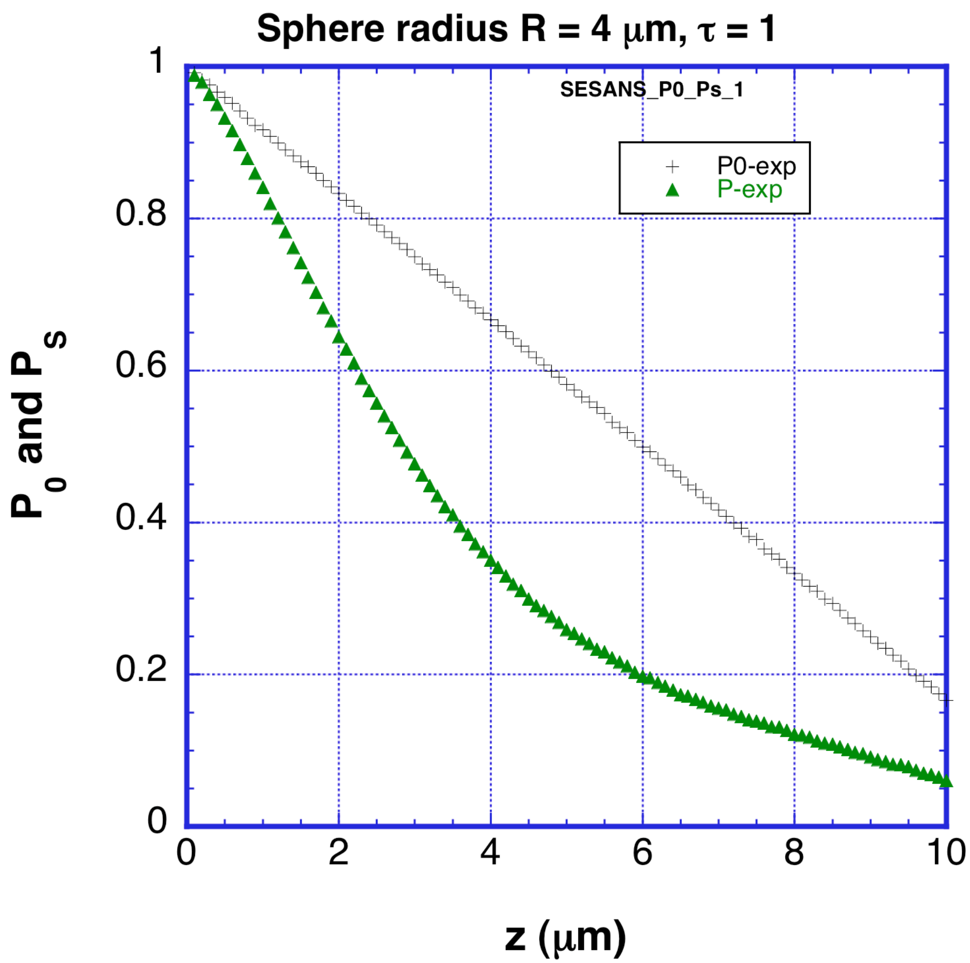
$$G(z) = \Re\left(\left[1 - \left(\frac{z}{2R}\right)^2\right]^{1/2}\left[1 + \frac{1}{2}\left(\frac{z}{2R}\right)^2\right] + 2\left(\frac{z}{2R}\right)^2\left(1 - \frac{z}{4R}\right)^2 \ln\left\{\frac{z/R}{2 + [4 - (z/R)^2]^{1/2}}\right\}\right), \tag{61}$$



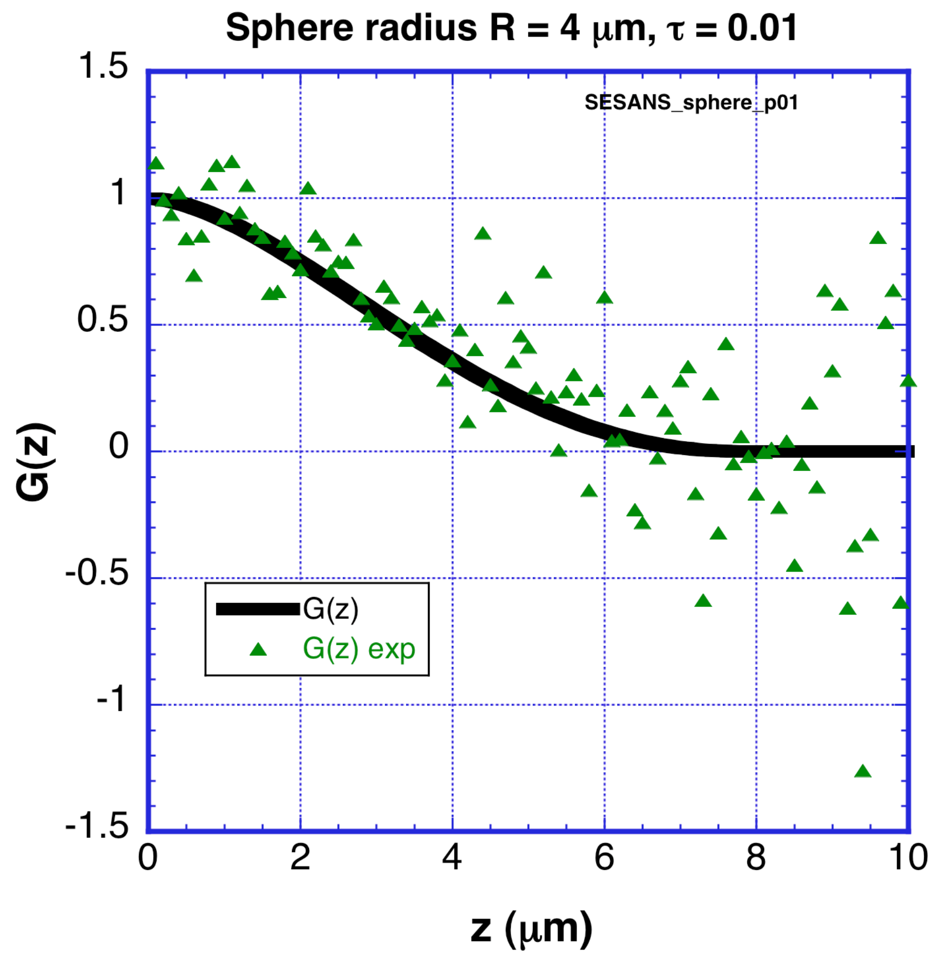
Correlation function or z projection
for 4 μm diameter spheres...
SESANS_cor_G
gamma(r)
G(z)
γ(r) or G(z)
r or z (μm)
0
0.2
0.4
0.6
0.8
1
0
2
4
6
8
10



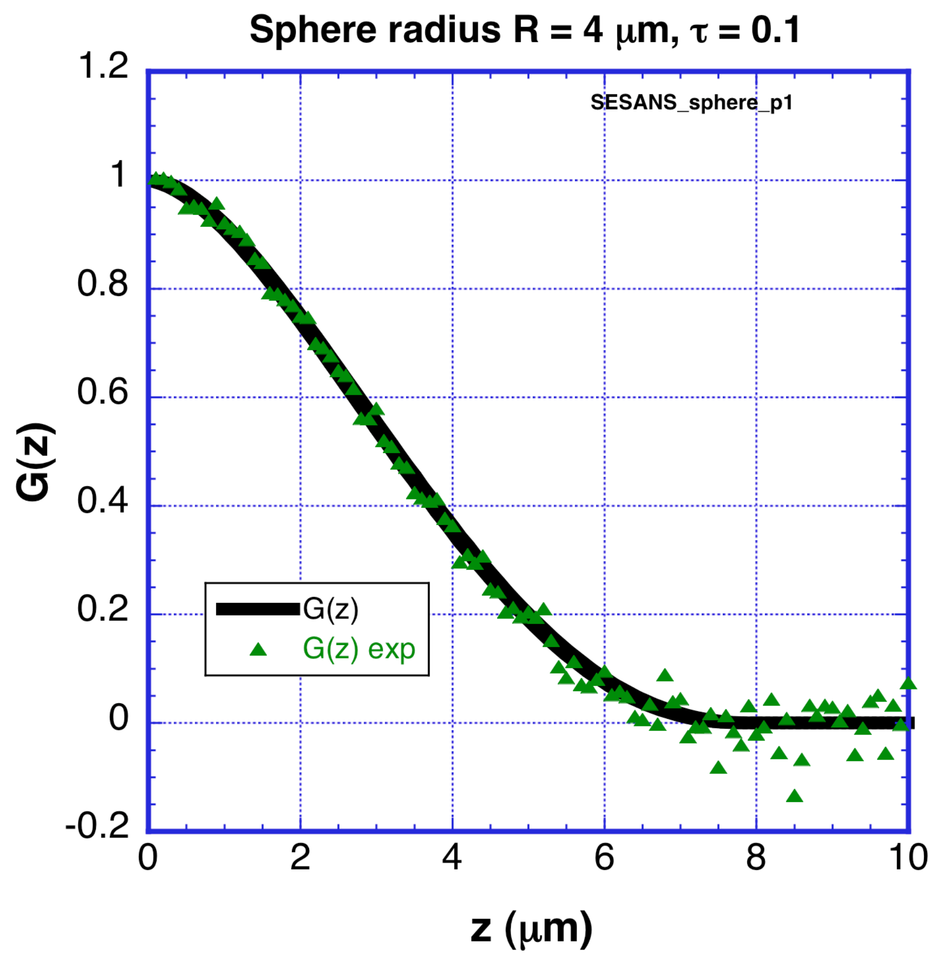
τ = 0.01
τ = 0.1
τ = 1
τ = 10
SESANS_Ps_P0
Unscattered Contribution
P_s / P_0
z (μm)
0
0.2
0.4
0.6
0.8
1
0
2
4
6
8
10



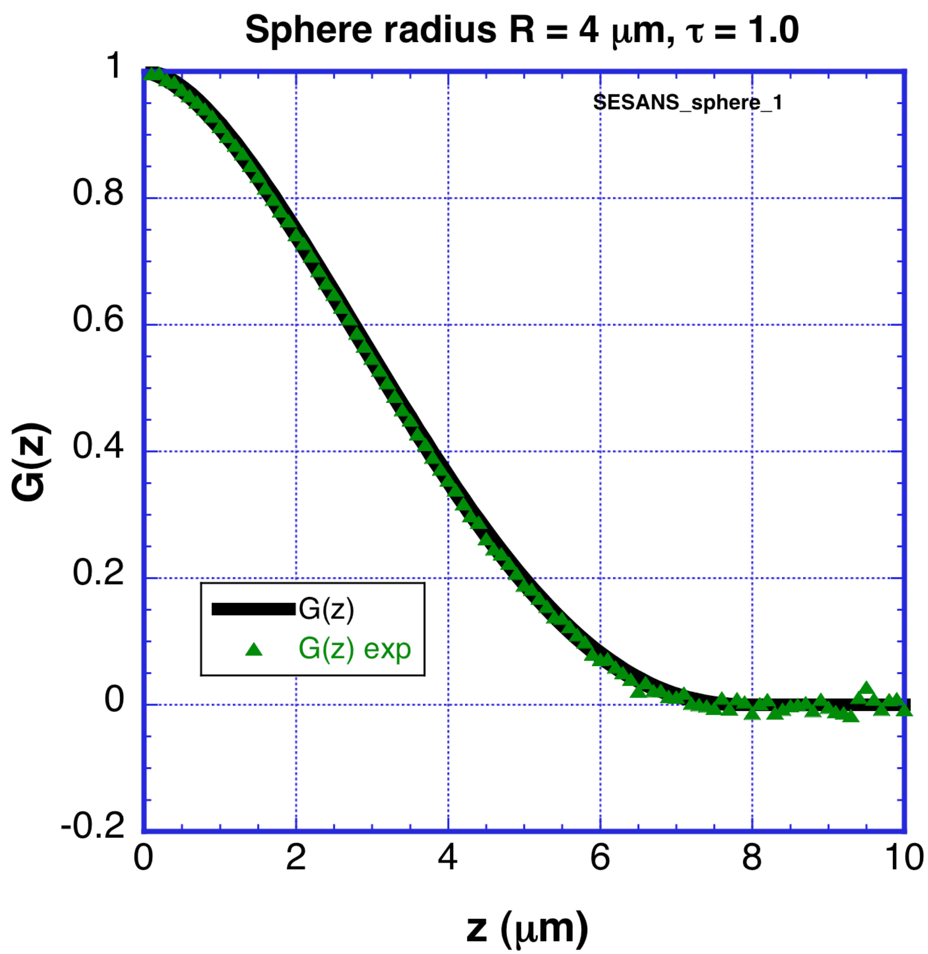
Sphere radius R = 4 μm, τ = 1
SESANS_P0_Ps_1
P0-exp
P-exp
P0 and Ps
z (μm)
0
0.2
0.4
0.6
0.8
1
0
2
4
6
8
10



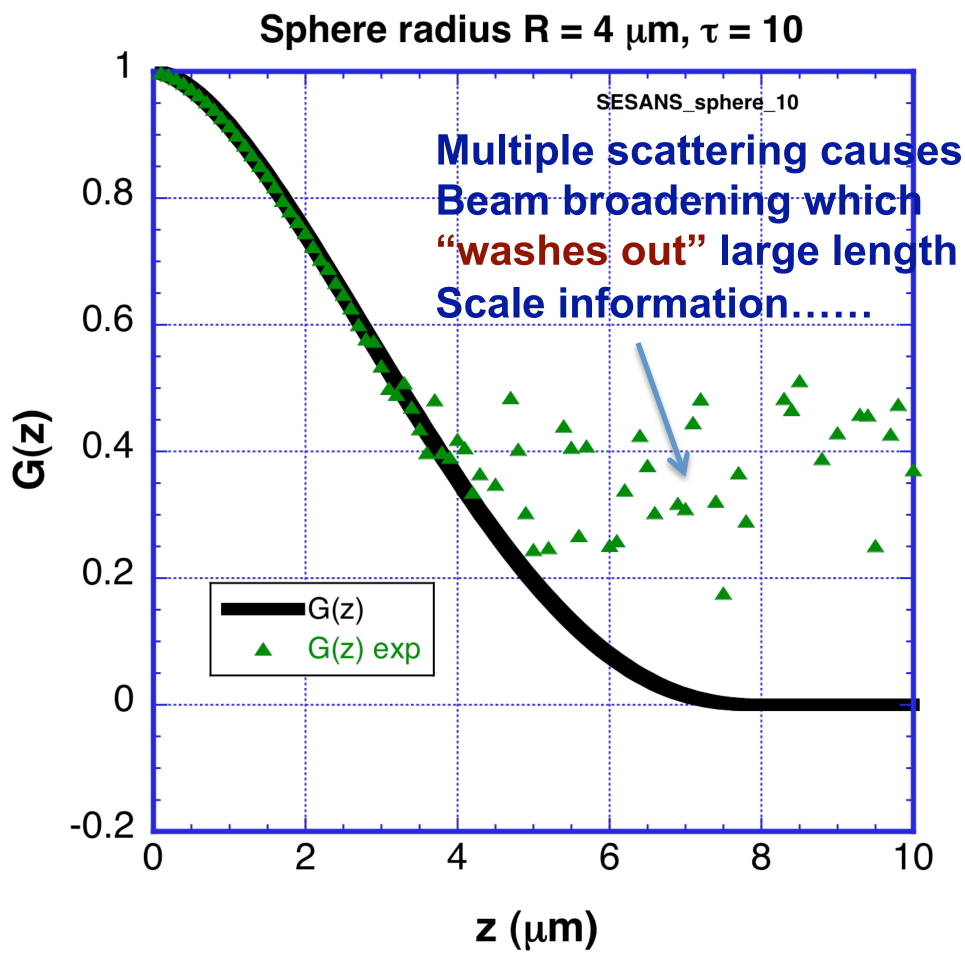
Sphere radius R = 4 μm, τ = 0.01
SESANS_sphere_p01
G(z)
G(z) exp
G(z)
z (μm)
1.5
1
0.5
0
-0.5
-1
-1.5
0
2
4
6
8
10



Sphere radius R = 4 μm, τ = 0.1
SESANS_sphere_p1
G(z)
G(z) exp
G(z)
z (μm)
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
0
2
4
6
8
10



Sphere radius R = 4 μm, τ = 1.0
SESANS_sphere_1
G(z)
G(z) exp
1
0.8
0.6
0.4
0.2
0
-0.2
0
2
4
6
8
10
z (μm)



Sphere radius R = 4 μm, τ = 10
SESANS_sphere_10
Multiple scattering causes
Beam broadening which
"washes out" large length
Scale information……
G(z)
G(z) exp
G(z)
z (μm)
1
0.8
0.6
0.4
0.2
0
-0.2
0
2
4
6
8
10

General Comments:

- Decoupling of angular resolution from “z” resolution allows faster data collection in USANS regime: $1 < z < 10$ microns

- But sensitivity degrades quickly for weak scatterers due to unscattered (empty) neutron contamination. Needs strong scattering samples!!! **Ideally, $0.5 \leq \tau \leq 2$**

- Further optimization of hardware is likely !!!
  - Improve polarization stability: Current 0.5 % to 0.1 % ??
  - Improve overall polarization at long z length scales:
    current $P = 0.3$ to $P >= 0.8$??

- TOF mode can quickly cover large z-range at high countrate
  - Allows rapid insitu measurements.
  - Possibly more stable echos…

Conclusions (or my crystal ball guesses of the future..)

- Instrument has a potential niche as a USANS instrument.
- But technique needs further development before making it a

  high performance alternative to Bonse-Hart type USANS.
- Does not require high flux neutron source. (ex: Pynn at LENS)
- Does require a stable magnetic environment.
- Considerable staff expertise and maintenance effort required…

  not likely to be a turn key user friendly instrument.
- TOF instrument at pulse source is best fit. (OFFSPEC at ISIS)
- Future SNS instrument after further development by

  Pynn at LENS or others elsewhere…