Methods that involve 2d-Fourier transformations in SANS:

multiple scattering and instrumental resolution

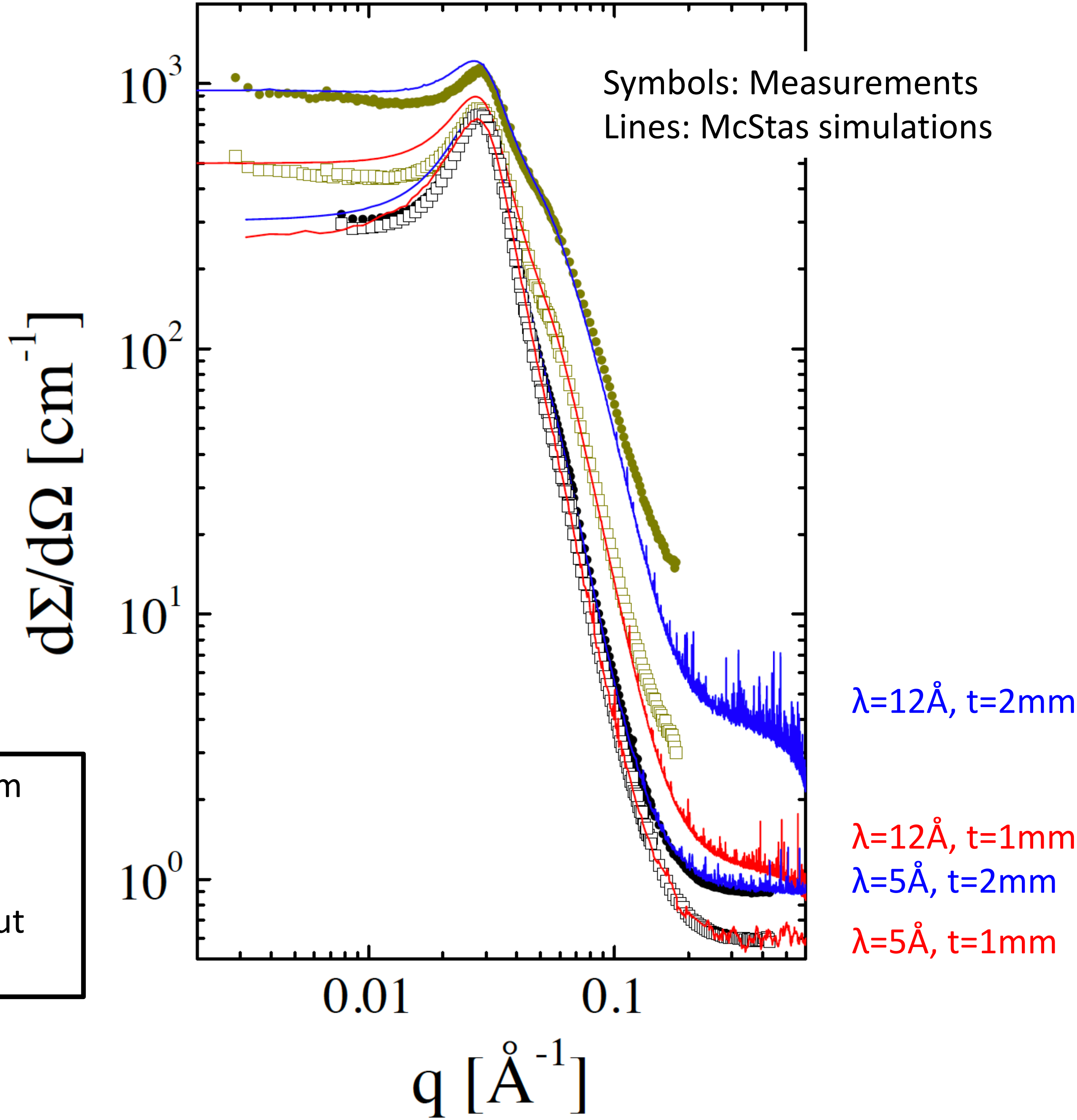
Henrich Frielinghaus

(NIMA Paper)

(Github: jugit.fz-juelich.de/sans/muscatt)

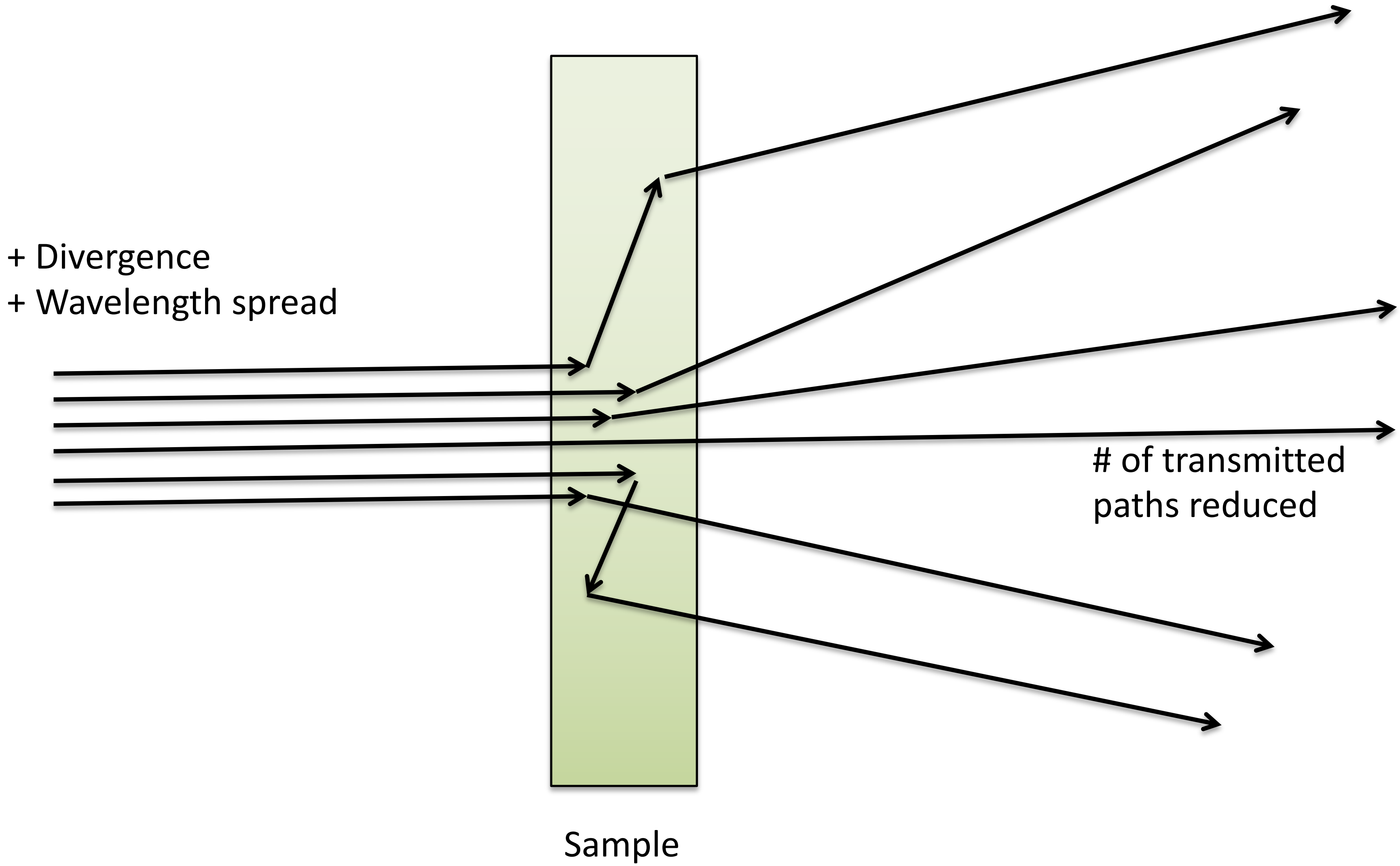
Microemulsions

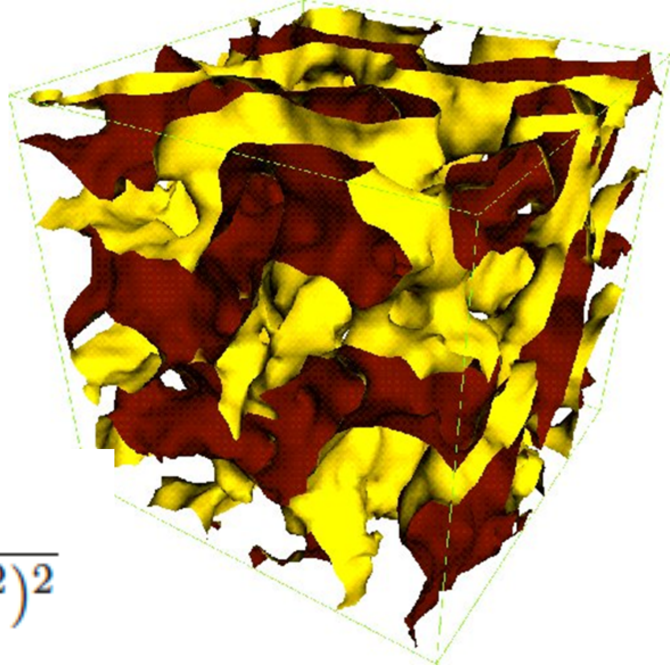
17%vol $C_{10}E_4$
41.5% D_2O
41.5% n-decane



Fit formula to 5Å, 1mm measurement. Then simulate other measurements without any free parameters.

Mc Stas Simulations



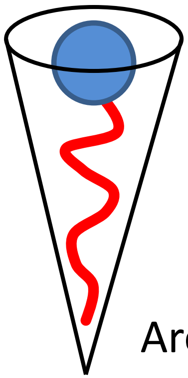


Low q-part:
smoothened interfaces

$$\frac{d\Sigma_c}{d\Omega}(q) = \Bigg(\frac{A_1}{q^4 - 2(k_0^2 - \xi^{-2})q^2 + (k_0^2 + \xi^{-2})^2} + \frac{A_2 \cdot \mathrm{erf}^{12}(1.06qR_g/\sqrt{6})}{q^4 R_g^4}\Bigg)\exp(-\sigma^2 q^2)$$

Additional surface due to
higher roughness

Film roughness

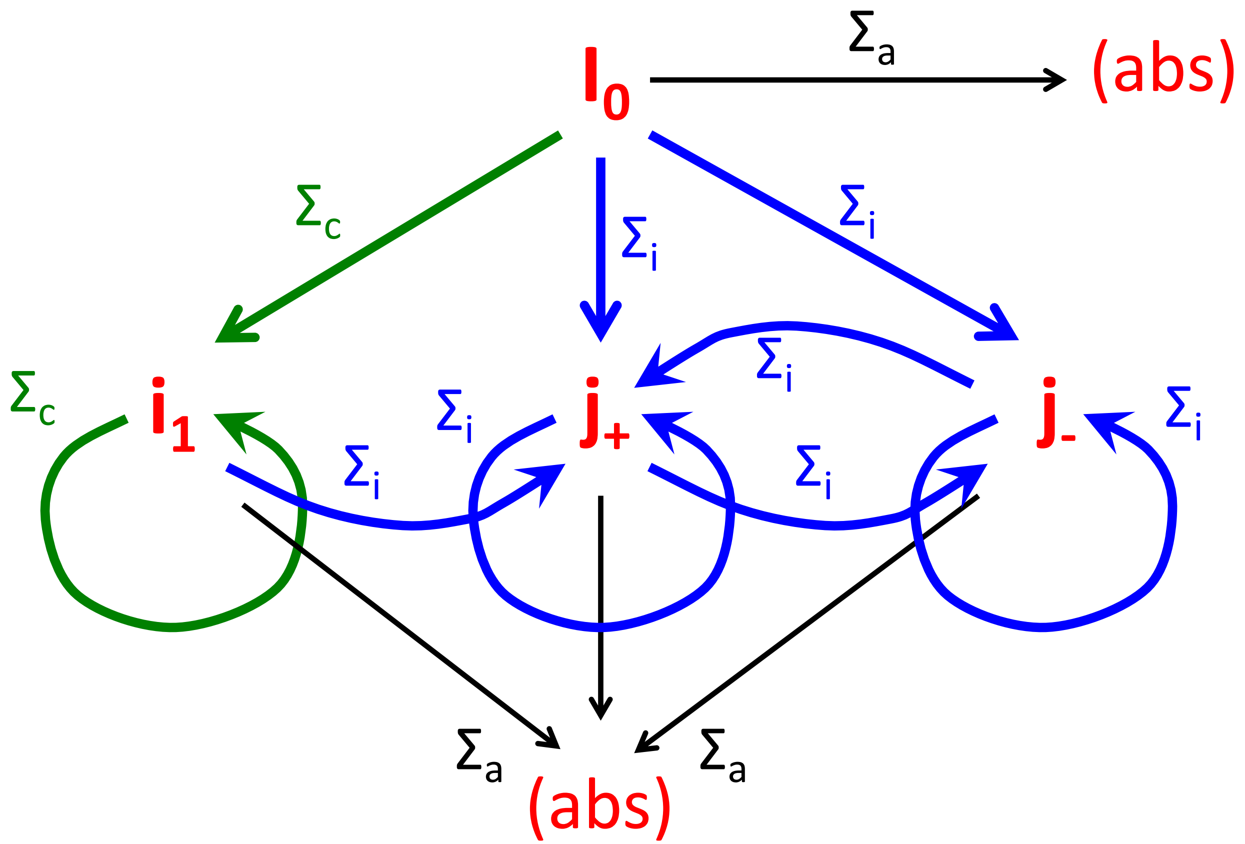


Area per head group might be wrong with multiple scattering

Analytical treatment of slab geometry

$$
\begin{aligned}
\partial_x I_0(x) &= -\Sigma_\mathrm{t} I_0(x) \\
\partial_x i_1(x,\mathbf{q}) &= \frac{d\Sigma_\mathrm{c}}{d\Omega}(\mathbf{q}) I_0(x) \\
&+ \int \frac{d\Sigma_\mathrm{c}}{d\Omega}(\mathbf{q}'-\mathbf{q}) i_1(x,\mathbf{q}') d^2\Omega' \\
&- \Sigma_\mathrm{t} i_1(x,\mathbf{q}) \\
\partial_x j_+(x,\vartheta) &= \frac{\Sigma_\mathrm{i}}{4\pi}\left(I_0(x)+I_1(x)+\int \frac{j_+ + j_-}{\cos\vartheta} d^2\Omega\right) \\
&- \Sigma_\mathrm{ia}\frac{j_+(x,\vartheta)}{\cos\vartheta} \\
-\partial_x j_-(x,\vartheta) &= \frac{\Sigma_\mathrm{i}}{4\pi}\left(I_0(x)+I_1(x)+\int \frac{j_+ + j_-}{\cos\vartheta} d^2\Omega\right) \\
&- \Sigma_\mathrm{ia}\frac{j_-(x,\vartheta)}{\cos\vartheta}
\end{aligned}
$$

Analytical treatment of slab geometry



Analytical solutions of slab geometry

$$I_0 = \hat{I}\exp(-\Sigma_\mathrm{t} x) \qquad T = \exp(-\Sigma_\mathrm{t} d)$$

$$I_1 = \hat{I}(-\exp(-\Sigma_\mathrm{t} x) + \exp(-\Sigma_\mathrm{ia} x))$$

Ideal thickness: $x = \ln(\Sigma_\mathrm{t}/\Sigma_\mathrm{ia})/\Sigma_\mathrm{c}$

Scattering signal:

$$\tilde{\imath}_1(d,r) = \hat{I}\frac{2\pi}{\lambda^2}\left(\exp\left(\frac{\lambda^2}{2\pi}\widetilde{\frac{d\Sigma_\mathrm{c}}{d\Omega}}(r)d\right) - 1\right)\exp(-\Sigma_\mathrm{t} d)$$

Also found by Schelten/Schmatz
and: Monkenbusch

Formal inversion:

$$\widetilde{\frac{d\Sigma_\mathrm{c}}{d\Omega}}(r) = d^{-1}\cdot\frac{2\pi}{\lambda^2}\cdot\ln\left(\frac{\lambda^2}{2\pi}\frac{\tilde{\imath}_1(d,r)}{\hat{I}Td}d + 1\right)$$

Analytical solutions of slab geometry

Formal inversion:

$$\frac{\widetilde{d\Sigma_{\rm c}}}{d\Omega}(r) = d^{-1} \cdot \frac{2\pi}{\lambda^2} \cdot \ln\left(\frac{\lambda^2}{2\pi}\frac{\tilde{\imath}_1(d,r)}{\hat{I}Td}d + 1\right)$$

Alternative:

$$\frac{\widetilde{d\Sigma_{\rm noncal}}}{d\Omega}(r) = \frac{\tilde{\imath}_1(d,0)}{T_{\rm ia} - T} \cdot \ln\left(\frac{\tilde{\imath}_1(d,r)}{\tilde{\imath}_1(d,0)}\frac{T_{\rm ia} - T}{T}\frac{1}{\tilde{R}_{\rm P}(r)} + 1\right)$$

$$T_{\rm ia} = \exp(-\Sigma_{\rm ia} d)$$

Background subtraction:

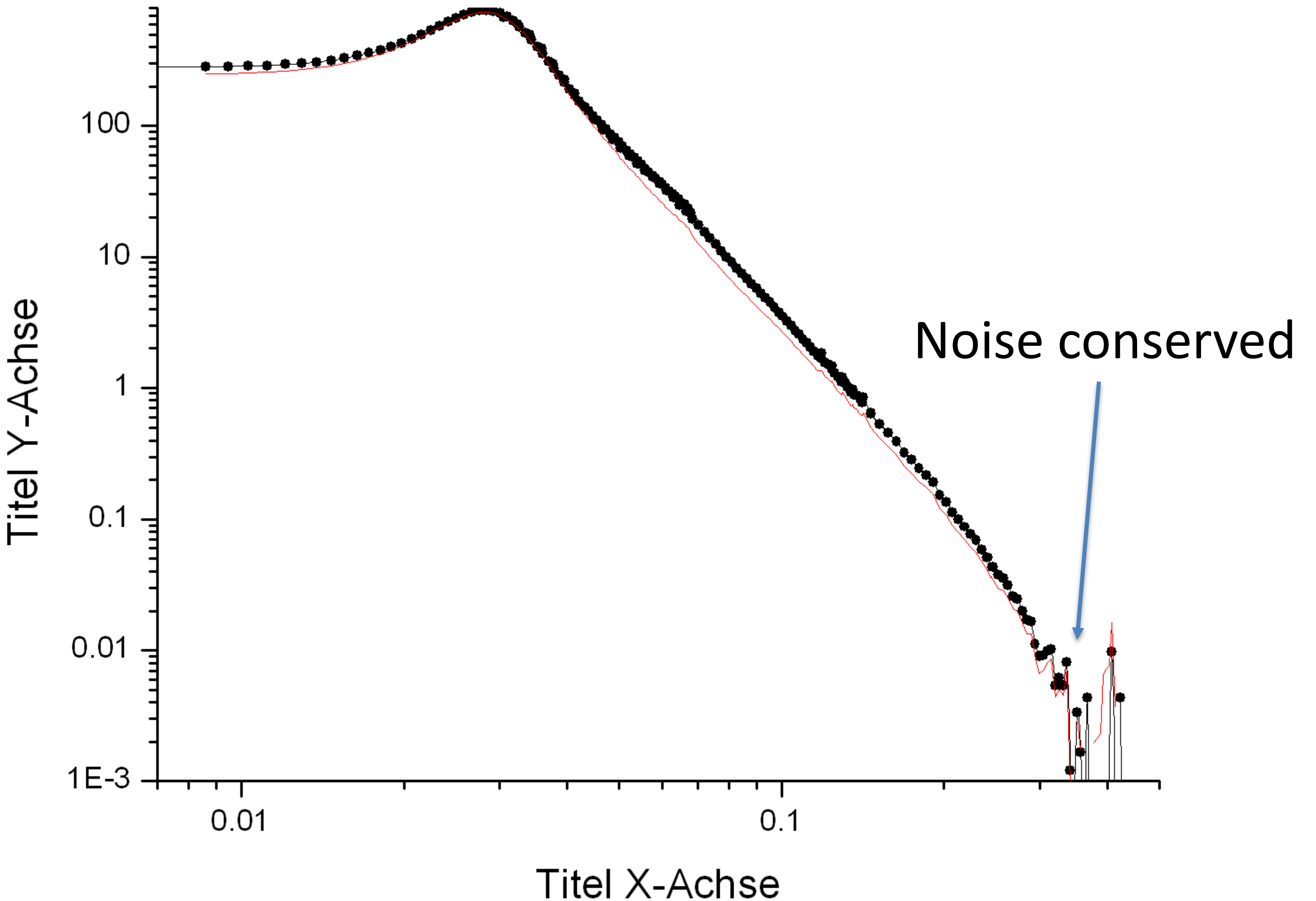
$$i_{\rm tot}(d, \langle\vartheta\rangle) = I_0(d)R(0,\vartheta) + i_1(d,q) \otimes R(\langle q\rangle, q) + j_+(d, \langle\vartheta\rangle)$$

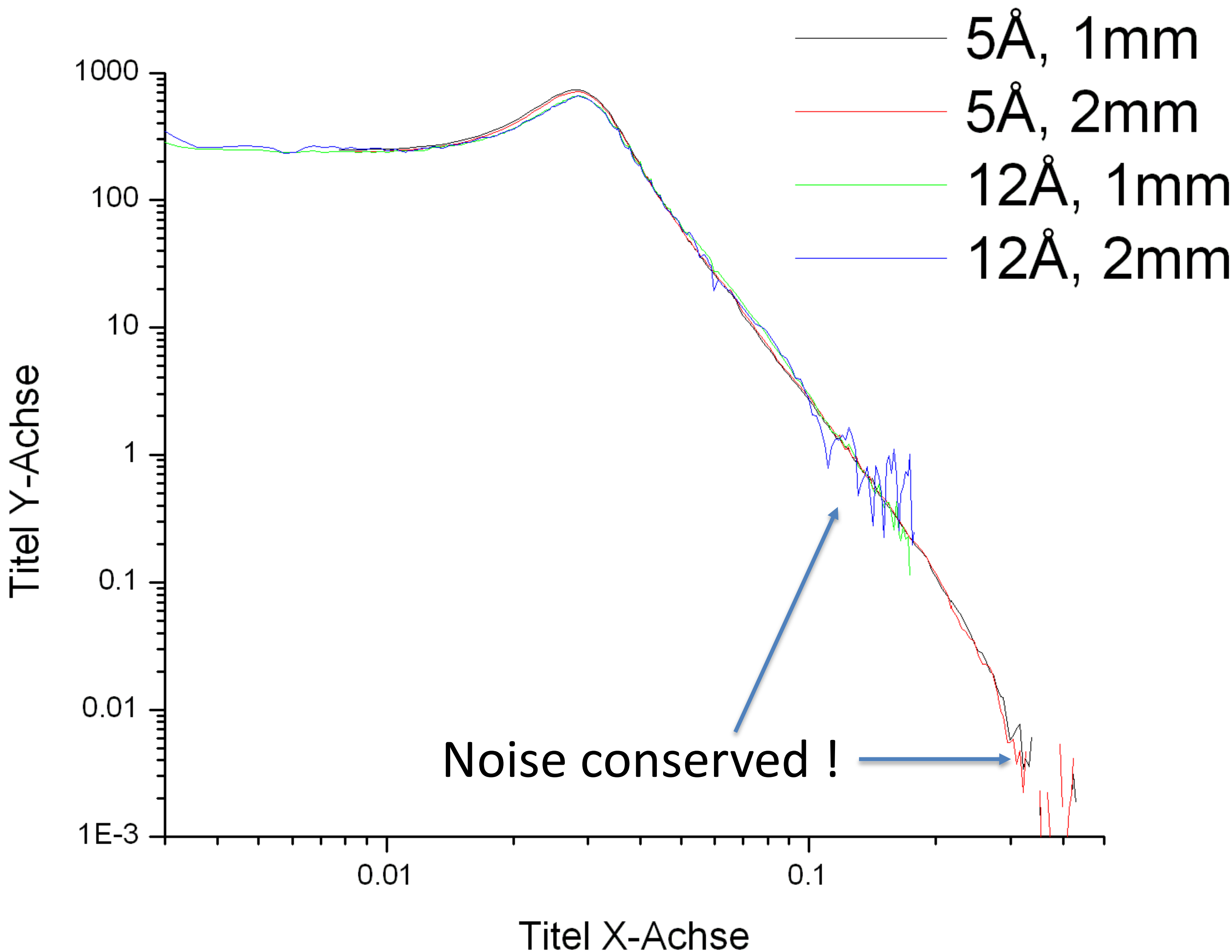
Primary beam

Incoherent bckgr.
can be experimental value

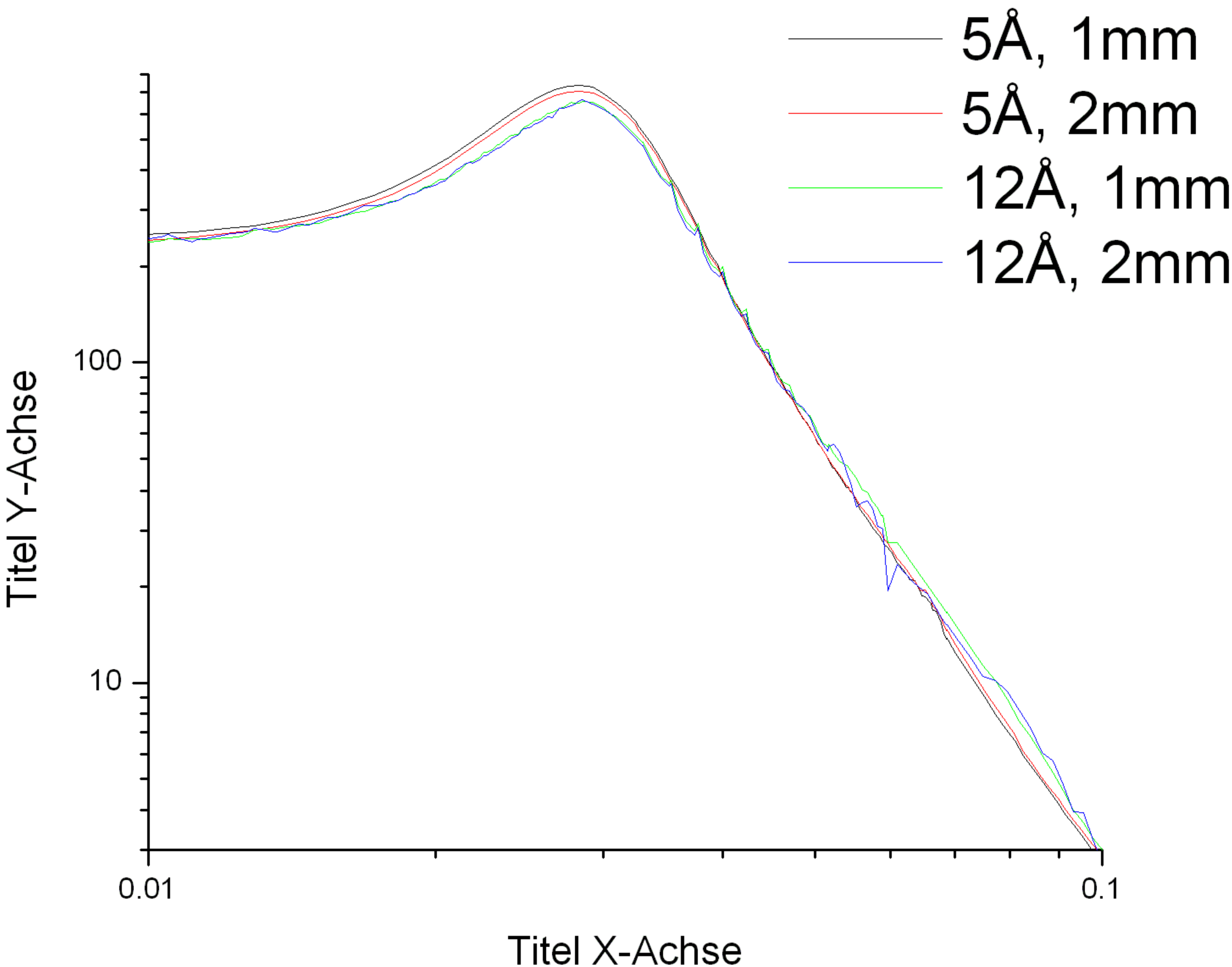
Strategy

- The transmission must be measured in the beam center using a reasonably high resolution to separate the coherent and incoherent scattering from the primary beam.
- The apparent scattering cross section is calibrated by dividing by the term $\hat{I}Td$.
- Usually several detector distances are combined to cover a large q-range.
- The incoherent background can be taken from experiments as a saturation level at reasonably high q. In some rare cases it might appear as a plateau.
- For the apparent coherent cross section the incoherent background level is subtracted.
- The removal of multiple scattering (and possibly resolution effects) is done using equation 10 or 11. The diligent experimentalist might want to try both ways to see whether his calibration was correct, but needs to look up the cross sections for incoherent scattering and absorption.
- The needed Hankel transformation (i.e. 2-dim. Fourier transformation of isotropic signals) may be done best by creating interpolation points on a logarithmic scale. In this way, the different detector distances may be represented best.
- The second Hankel transformation is performed in the same manner.


Noise conserved !
Titel Y-Achse
Titel X-Achse
100
10
1
0.1
0.01
1E-3
0.01
0.1



5Å, 1mm
5Å, 2mm
12Å, 1mm
12Å, 2mm
1000
100
10
1
0.1
0.01
1E-3
Titel Y-Achse
0.01
0.1
Titel X-Achse
Noise conserved !



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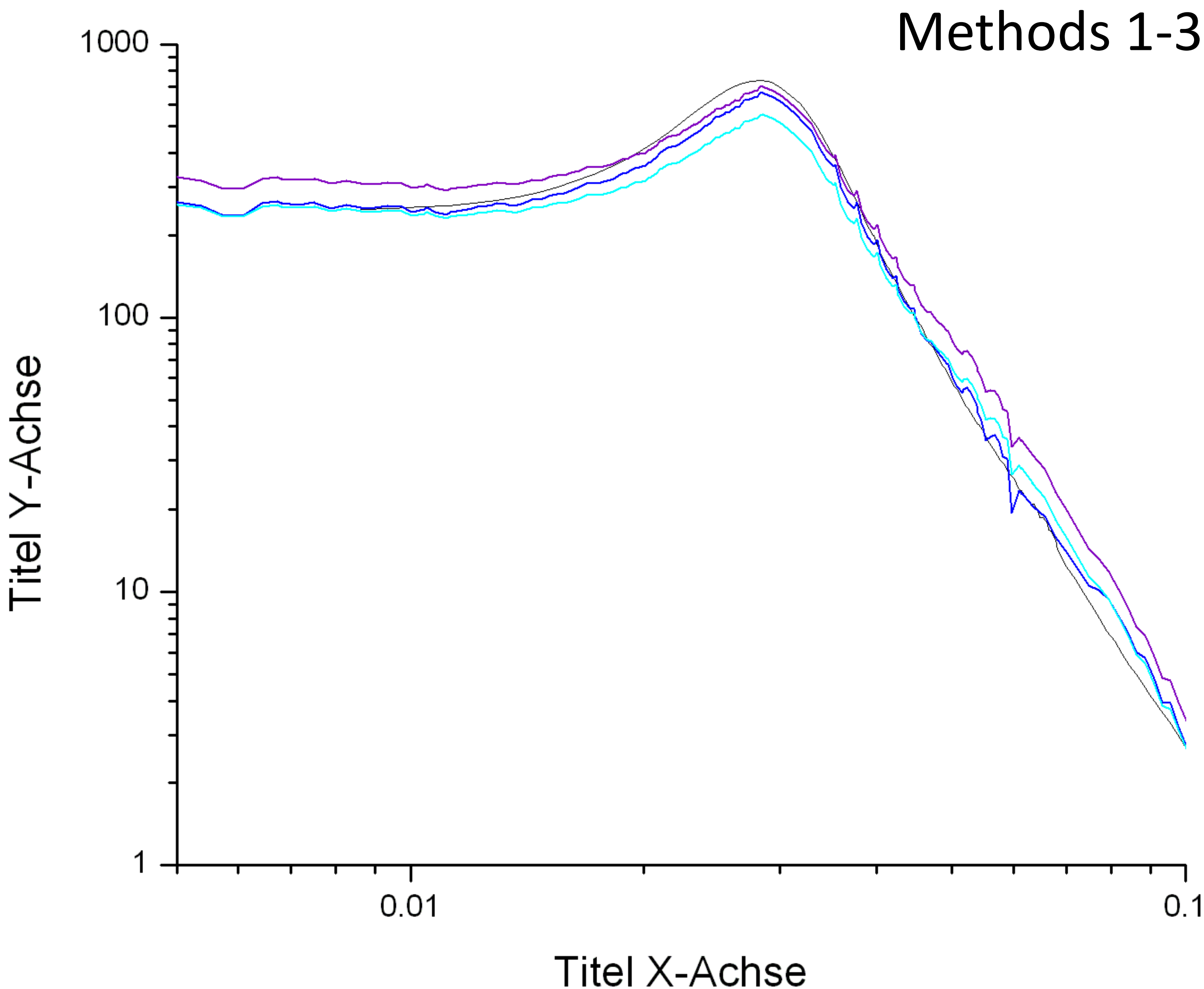
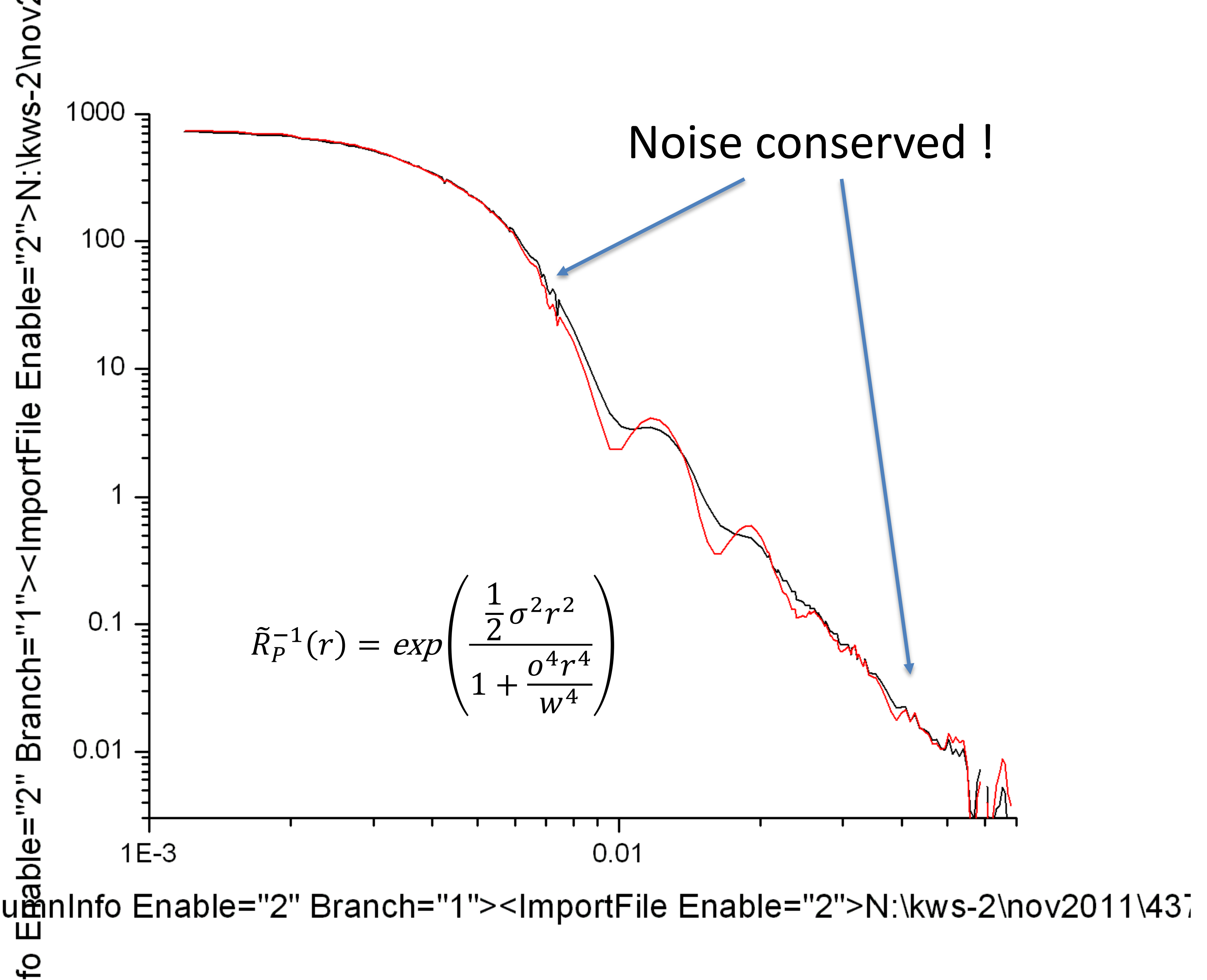
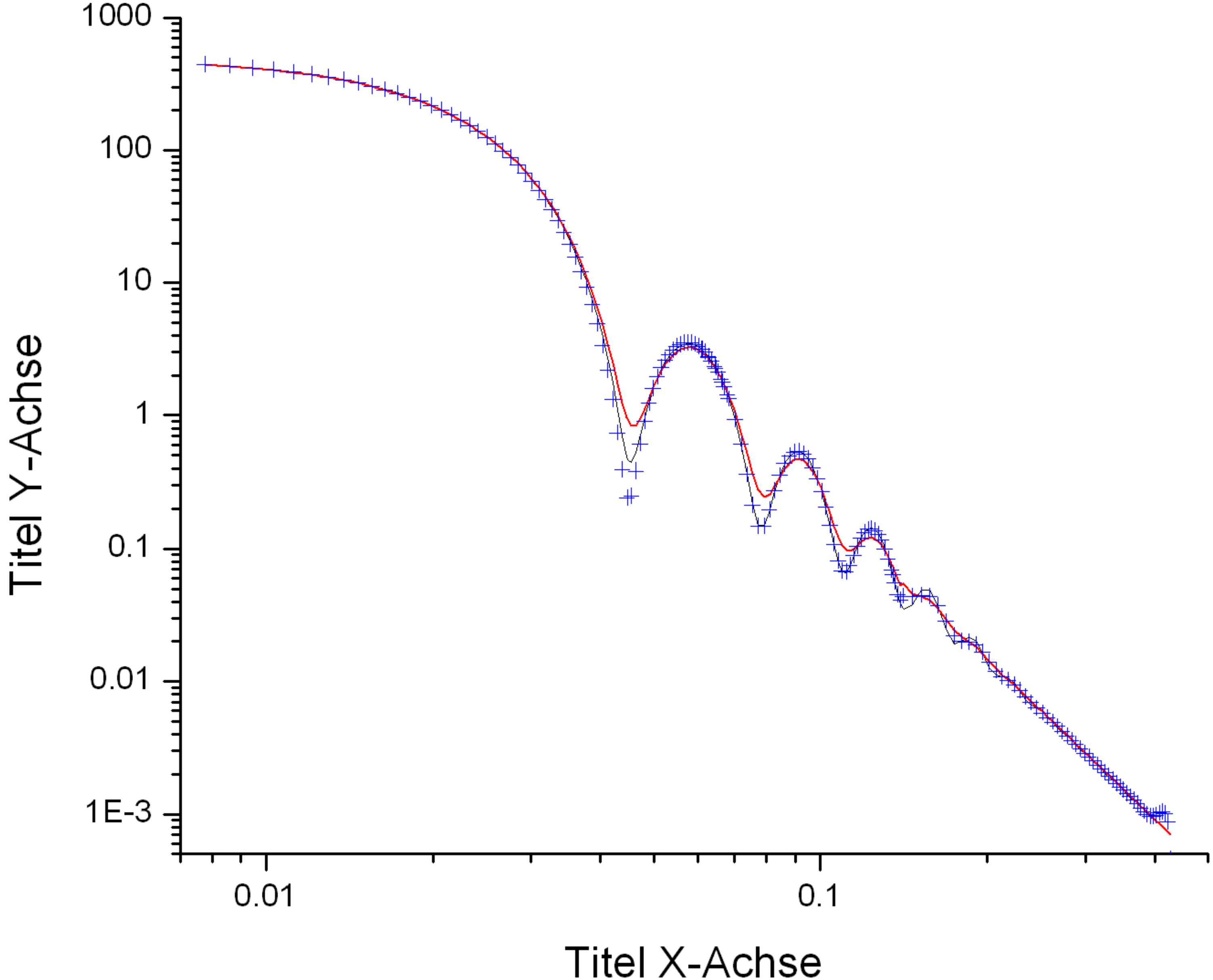


Methods 1-3
1000
100
10
1
0.01
0.1
Titel Y-Achse
Titel X-Achse

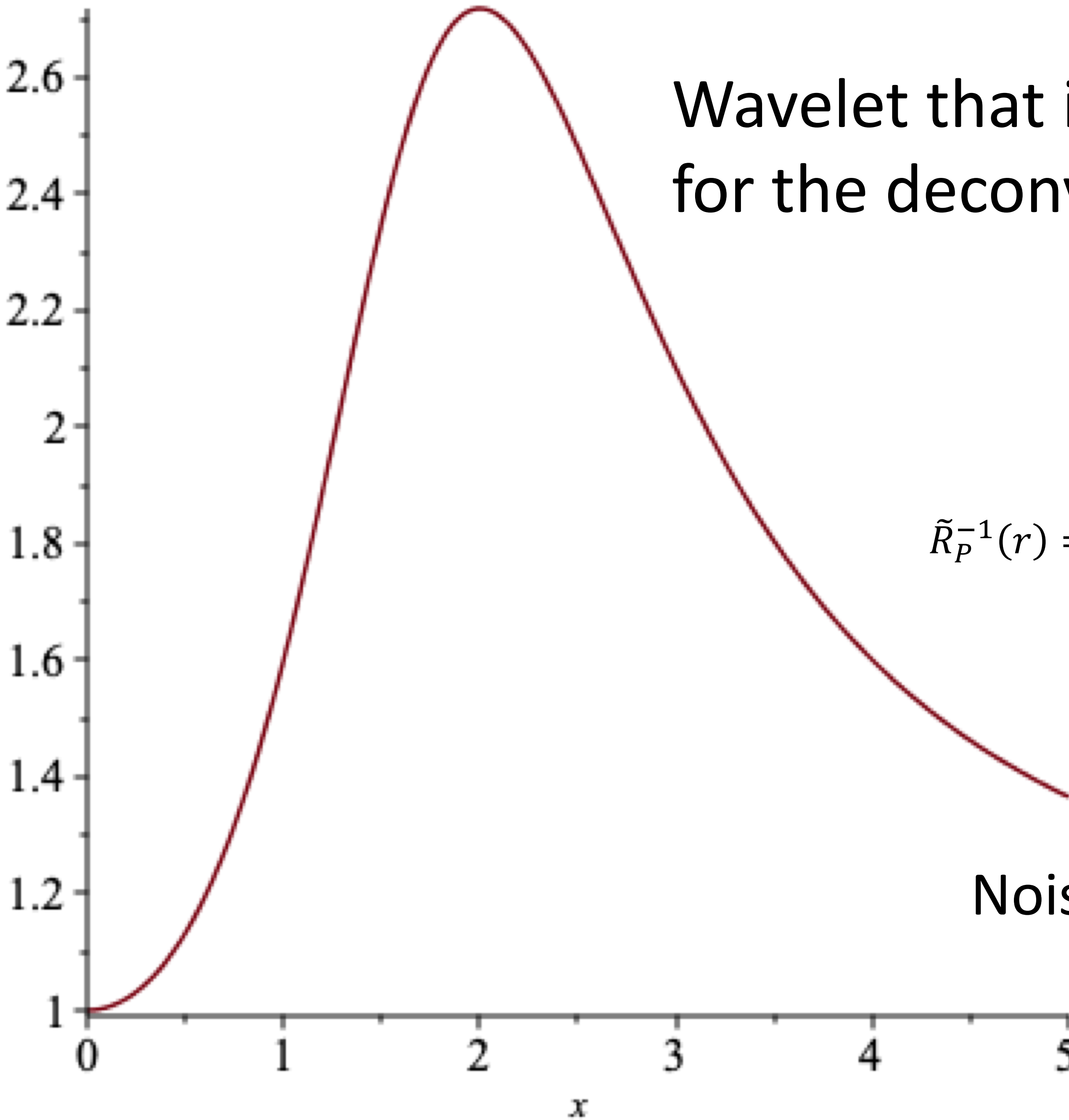


$$\tilde{R}_P^{-1}(r) = exp\left(\frac{\frac{1}{2}\sigma^2 r^2}{1 + \frac{o^4 r^4}{w^4}}\right)$$



1000
100
10
1
0.1
0.01
1E-3
0.01
0.1
Titel Y-Achse
Titel X-Achse

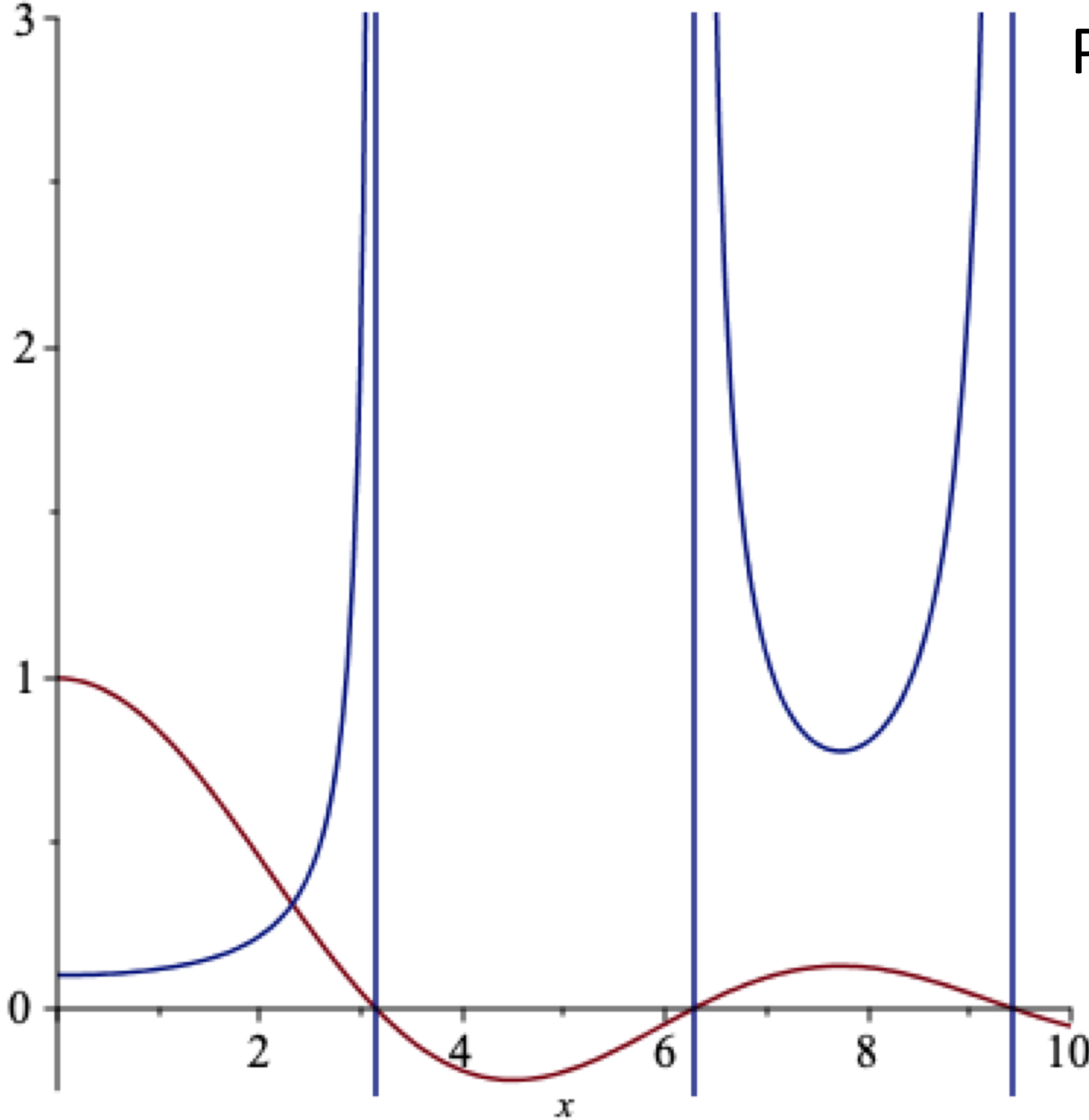
Wavelet that is used for the deconvolution

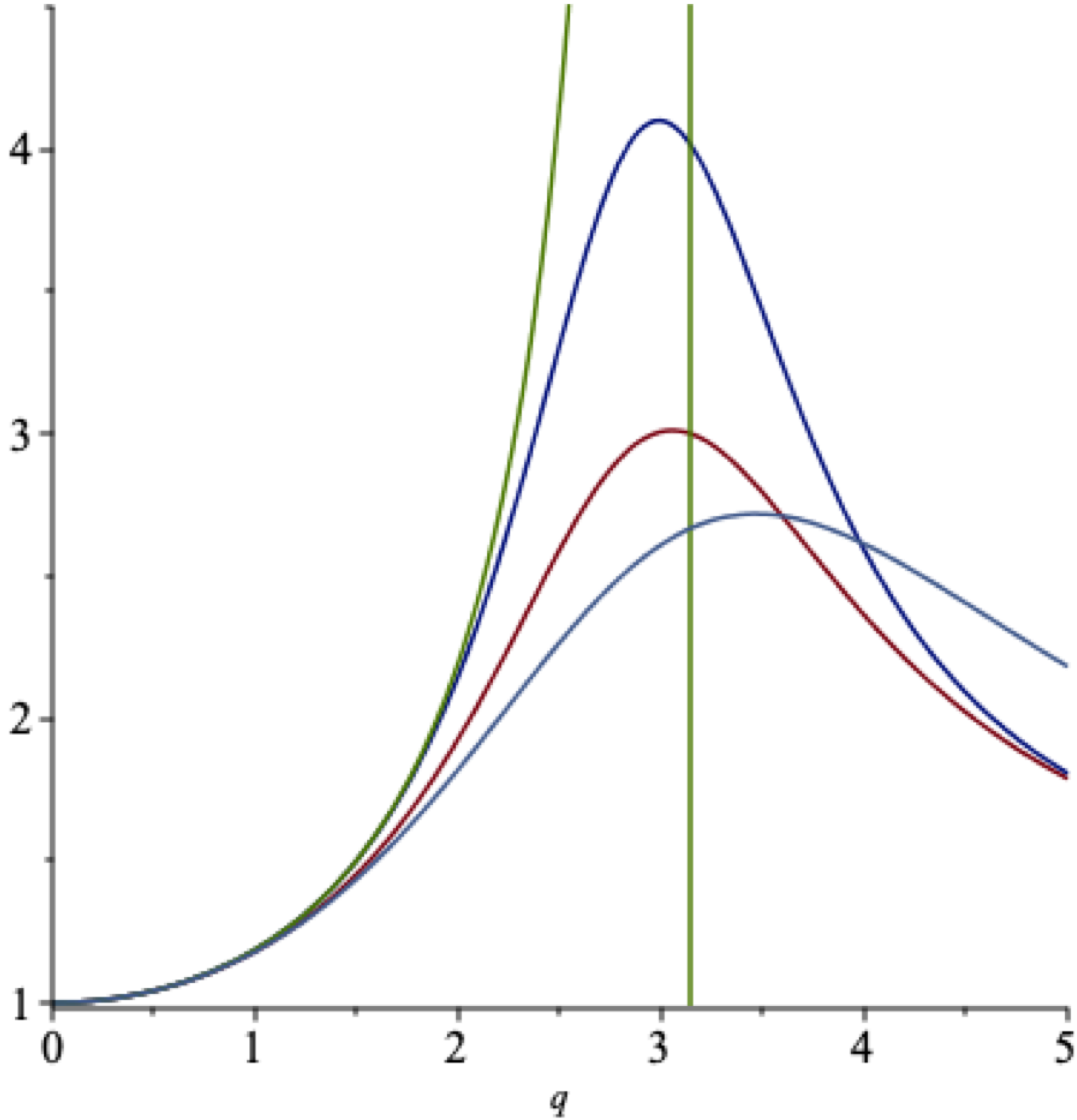


$$\tilde{R}_P^{-1}(r) = exp\left(\frac{\frac{1}{2}\sigma^2 r^2}{1 + \frac{o^4 r^4}{w^4}}\right)$$

Noise conserved !

Perfect Slit





4
3
2
1
0
1
2
3
4
5
q

What I see it can be used for:

- TOF SANS instruments: multiple scatt. & resolution
- Finite slit geometries: have unsymmetric resolution (also need for 2d detector image)