FIRST RESULTS FROM THE REFURBISHED J-NSE SPECTROMETER WITH SUPERCONDUCTING COILS

APRIL 2018 I M. MONKENBUSCH

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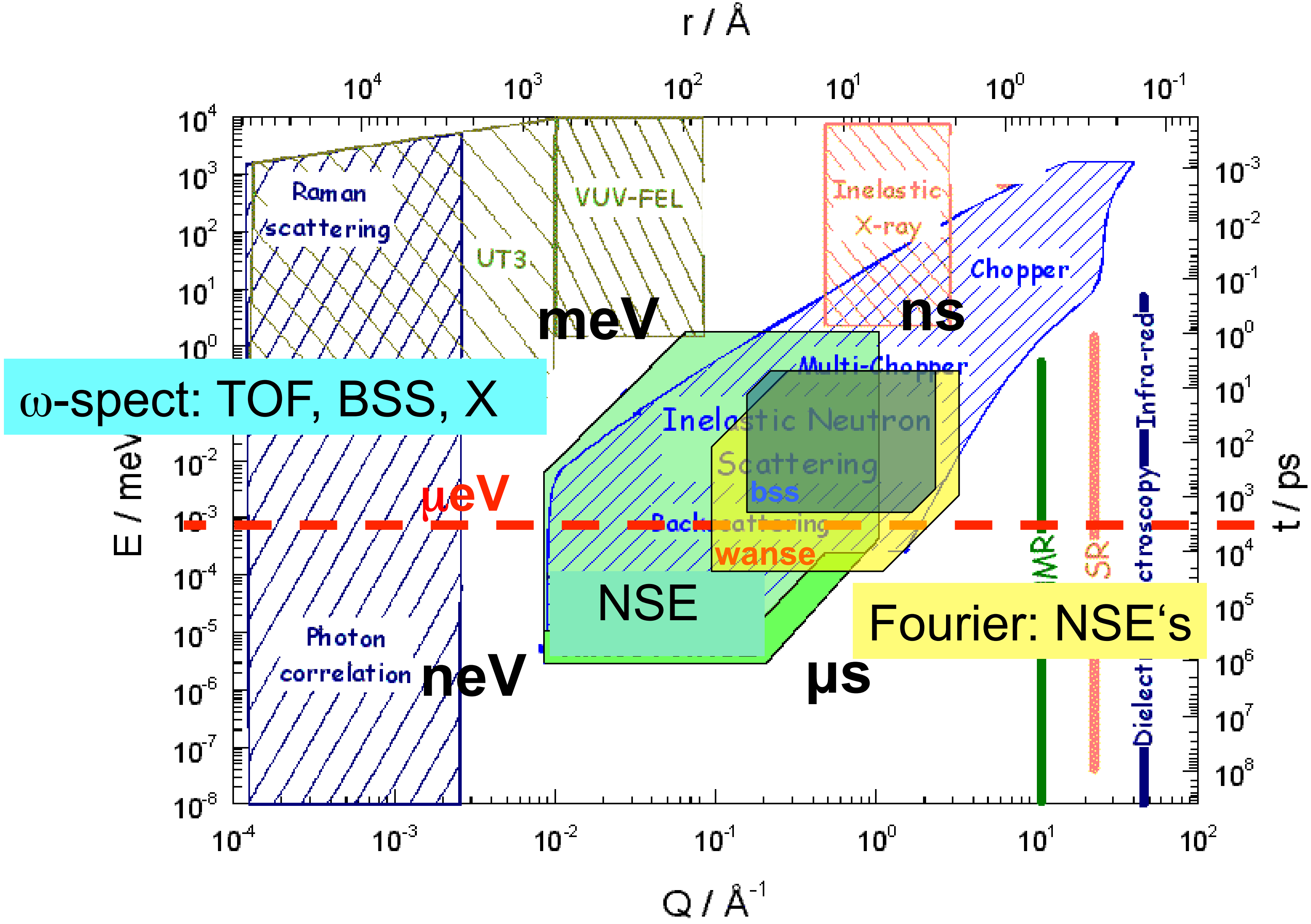
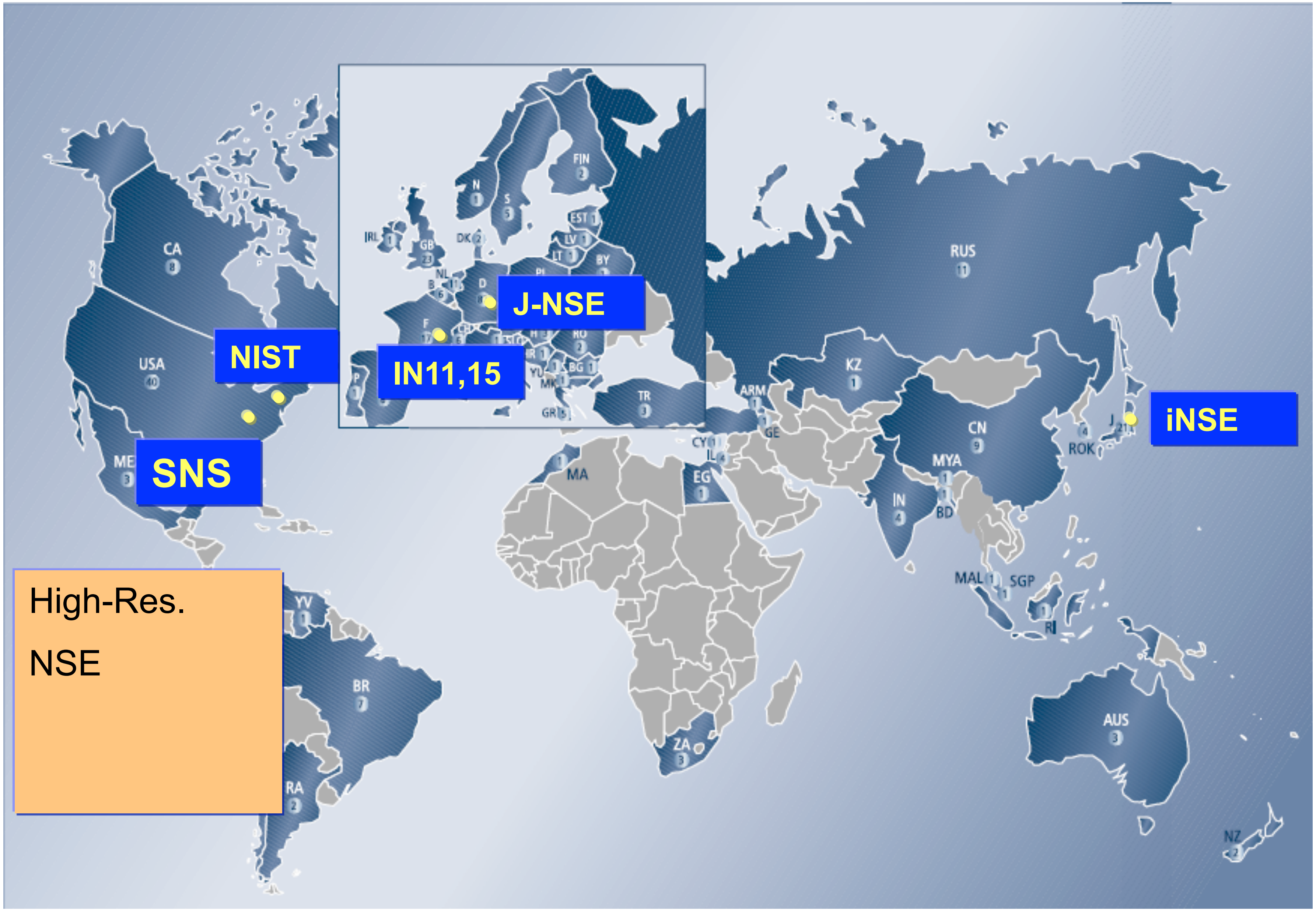
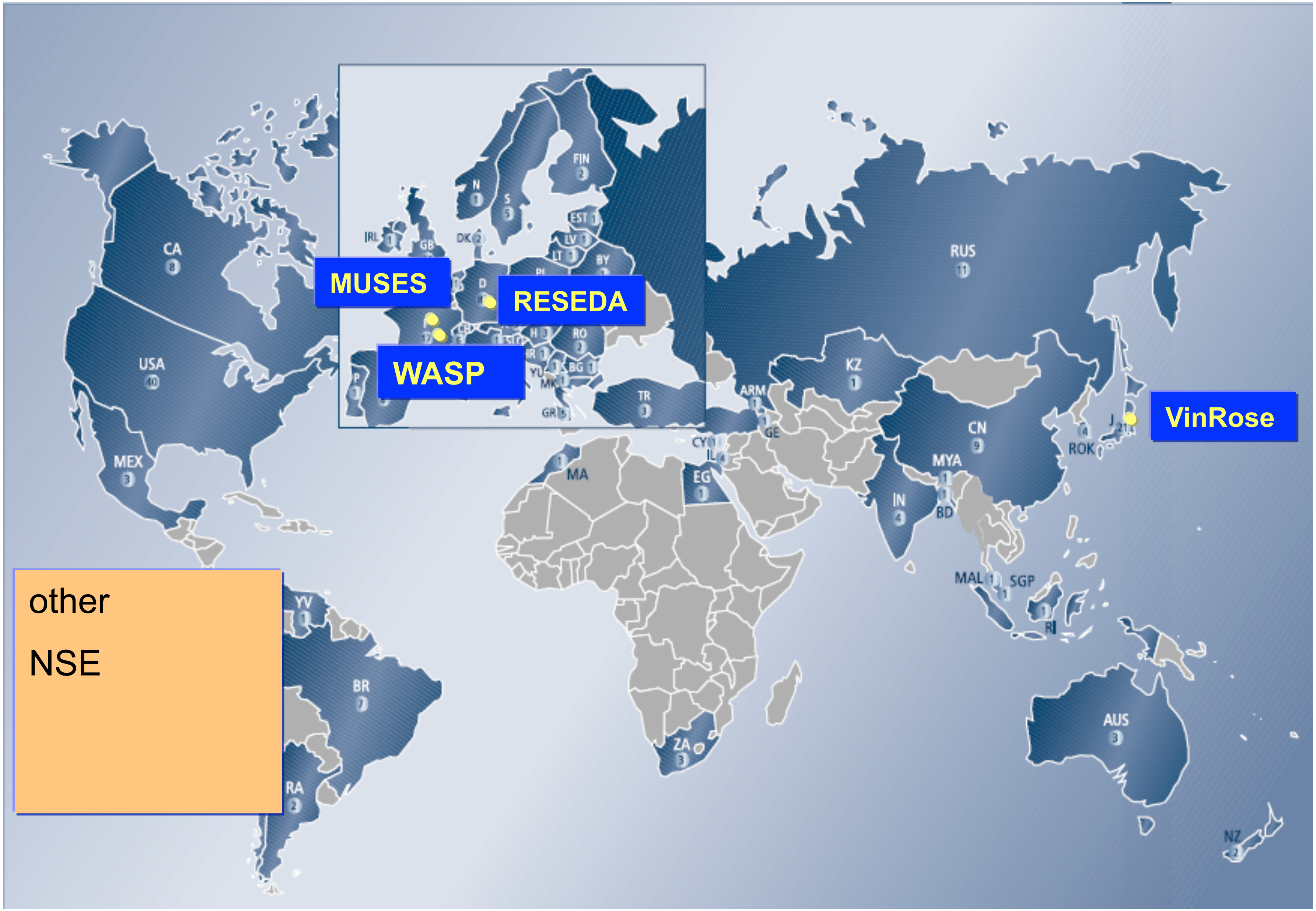
THE REALM OF NEUTRON SPIN ECHO



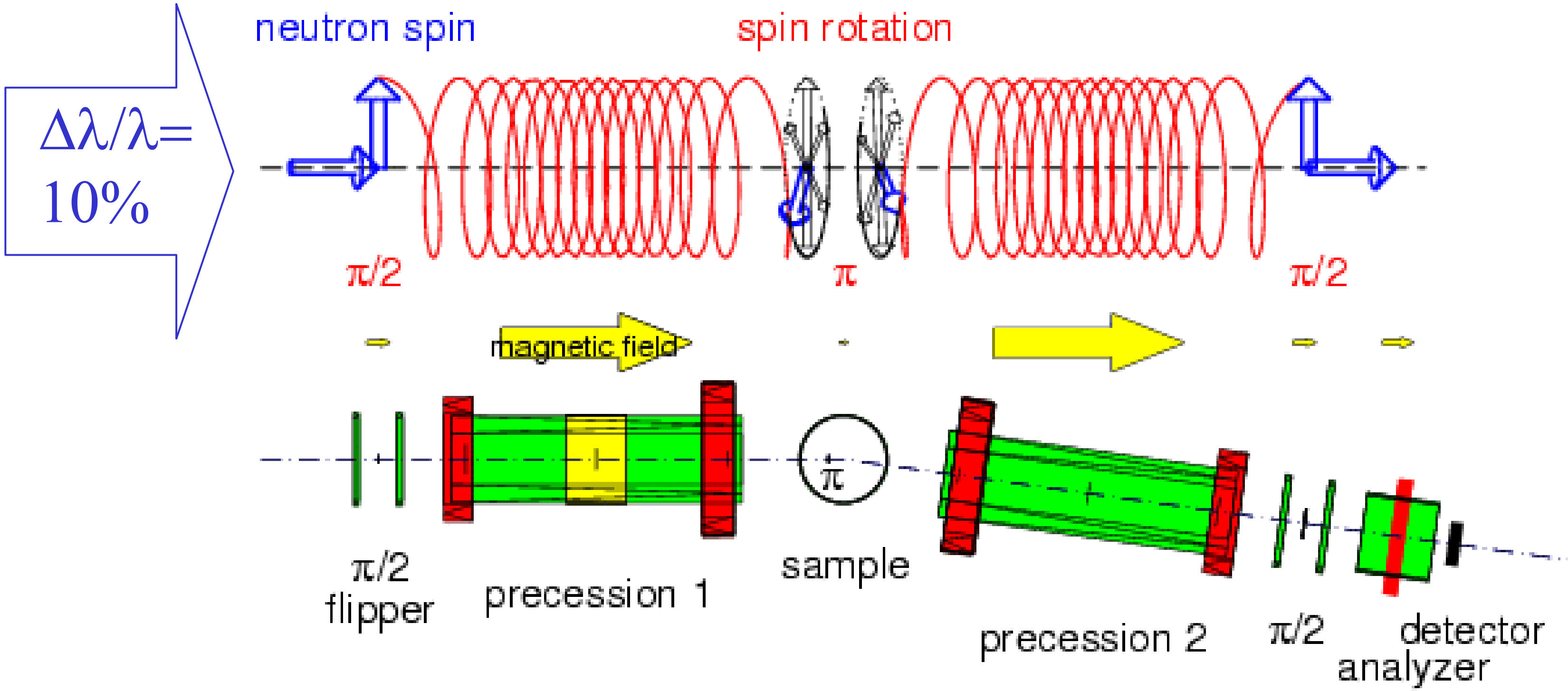
High-Resolution NSE worldwide

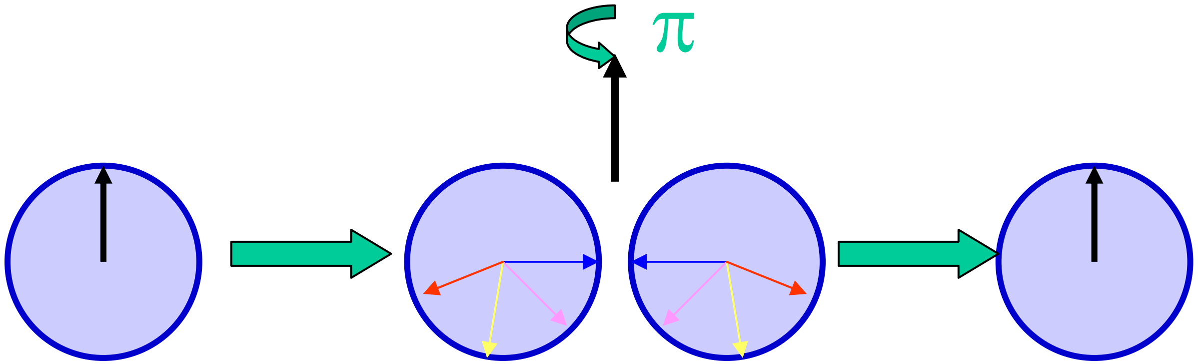


Medium-Resolution NSE worldwide



NSE spectrometer: (elastic scattering)

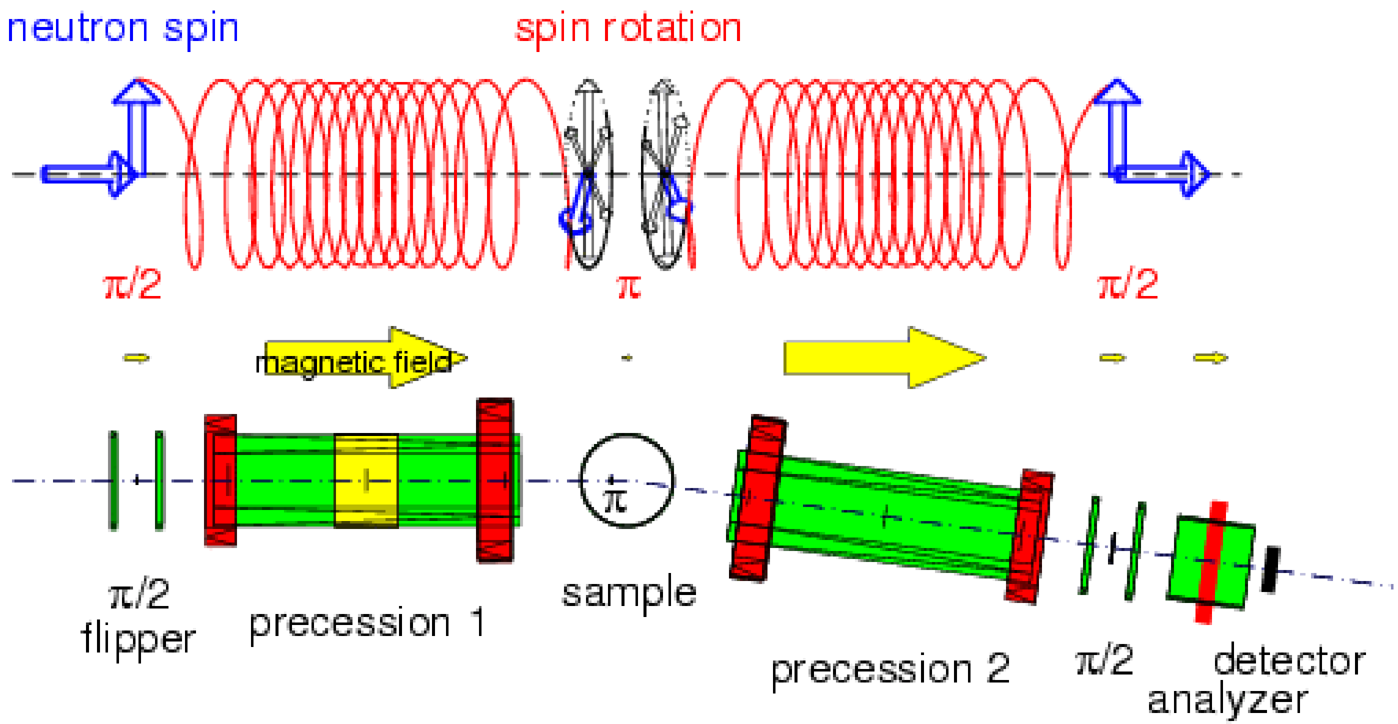


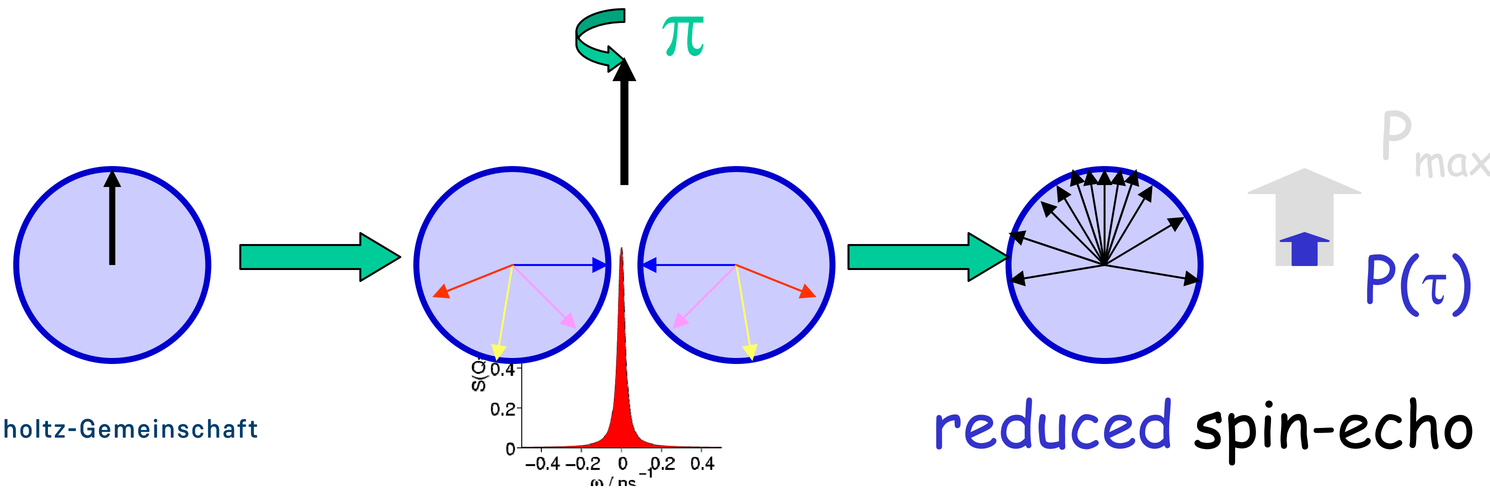


spin-echo

NSE spectrometer: (quasielastic scattering)

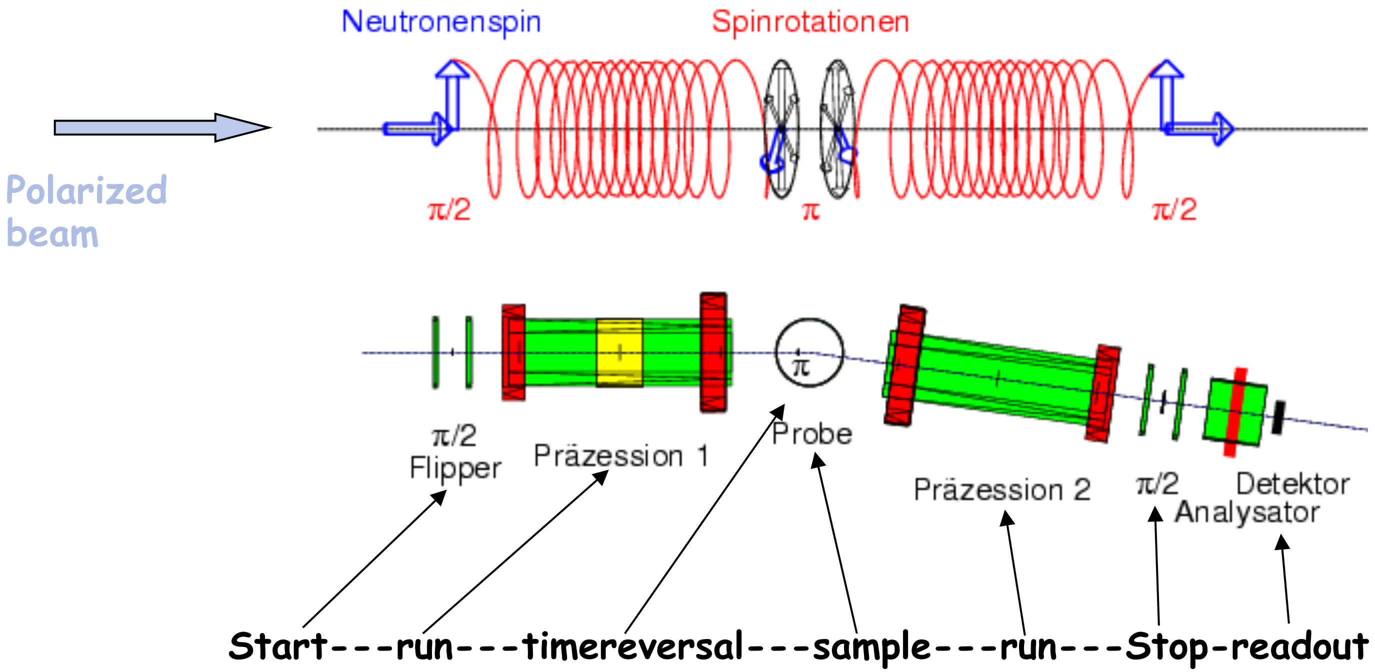
$\Delta\lambda/\lambda=$ 10%

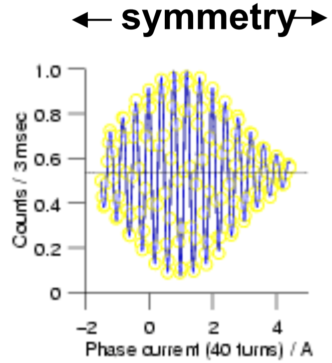




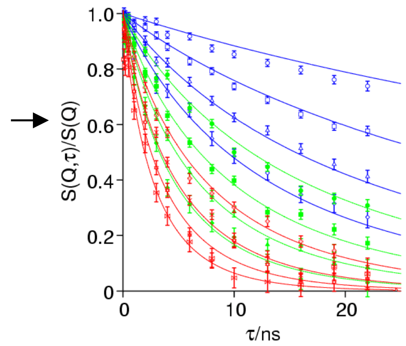
reduced spin-echo

Principle of NSE : Summary





Echoform

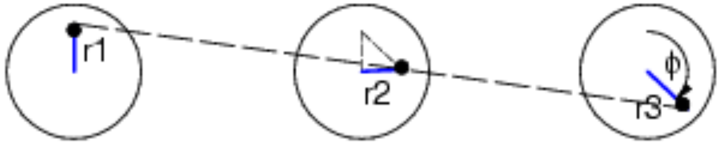


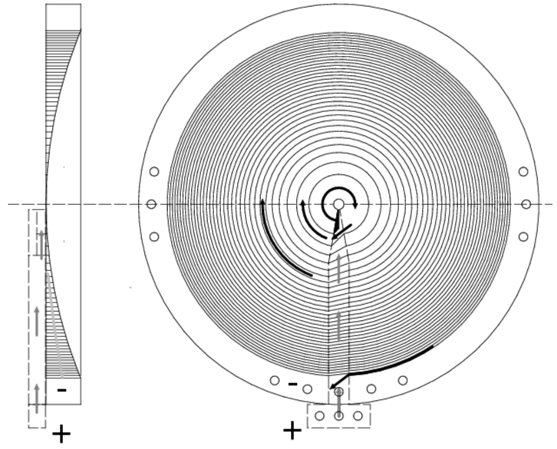
States of the indivdual spin-clocks

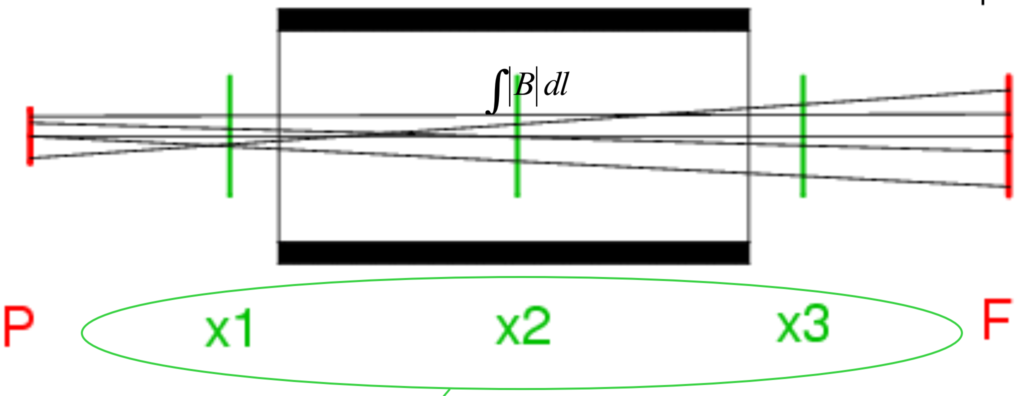
$$\tau \sim \lambda^3 \text{ “B L”}$$

"homogeneity" of field integrals determines the resolution

$$\int_{path} |B| \, dl$$

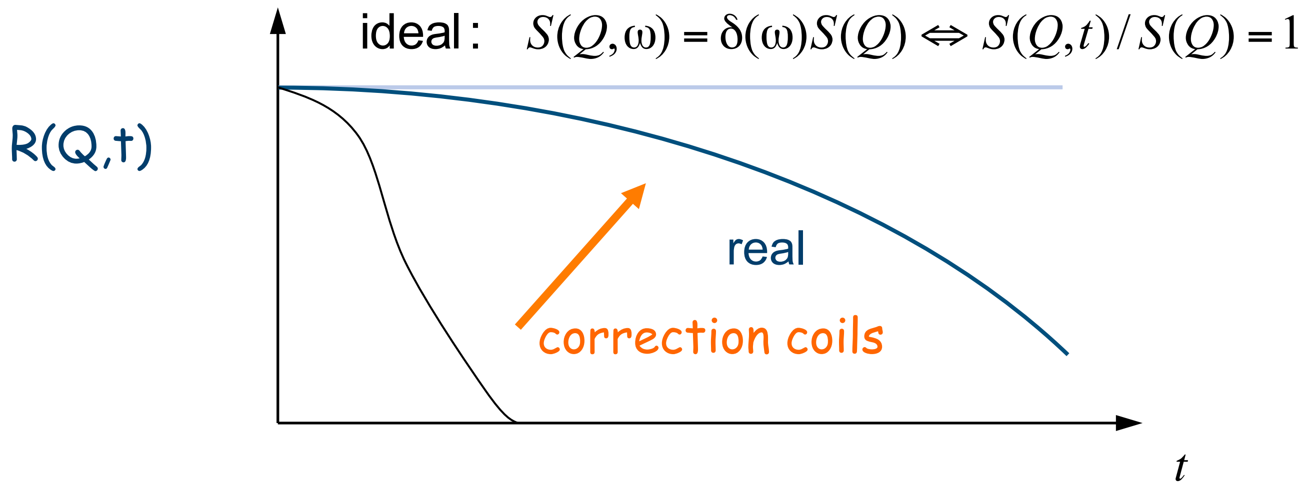






Three radial correction elements will do the job

Resolution correction



$$I = \eta\frac{1}{2}\left[S(Q) + \underbrace{\int \cos(\underbrace{\gamma J \frac{m_n^2}{h^2 2\pi}\lambda^3}_{t}\ \omega) S(Q,\omega) d\omega}_{S(Q,t)}\right]$$

R(Q,t)

Ansatz [Zeyen & Rem]:

$$B_z(z,r) = B_z(z,0) - \frac{1}{4} r^2 \partial_z^2 B_z(z,0) + O(r^4)$$

$$B_r(z,r) = -\frac{1}{2} r \partial_z B_z(z,0) + O(r^3).$$

$$J = \sqrt{1+\tan^2\theta} \int_{-L/2}^{L/2} \mathrm{d}z \, \left[B_z(z) + r^2 \underbrace{\left\{ \frac{1}{8} \frac{(\partial_z B_z(z))^2}{B_z(z)} - \frac{1}{4} \partial_z^2 B_z(z) \right\}}_{\beta(z)} \right] + \mathcal{O}\left(r^4\right),$$

$$J = J_0 + H r_0^2 + G \tan^2 \theta$$

$$J_0 = \int_{-L/2}^{L/2} \mathrm{d}z \; B_z(z),$$

$$H = \int_{-L/2}^{L/2} \mathrm{d}z \; \beta(z),$$

$$G = \frac{J_0}{2} + \int_{-L/2}^{L/2} \mathrm{d}z \; z^2 \beta(z).$$

Minimize!

$$\langle \Delta J[B(z)] \rangle = \langle \left(\sqrt{1+\tan^2\theta} - 1 \right) \rangle J_0 + \langle \sqrt{1+\tan^2\theta} \int_{-L/2}^{L/2} r(z)^2 \beta(z) \mathrm{d}z \rangle$$
$$\simeq \langle \tan^2\theta \rangle \; G + \langle r_0^2 \rangle \; H + \langle 2 r_0 \tan\theta \rangle \; U, \qquad (15)$$

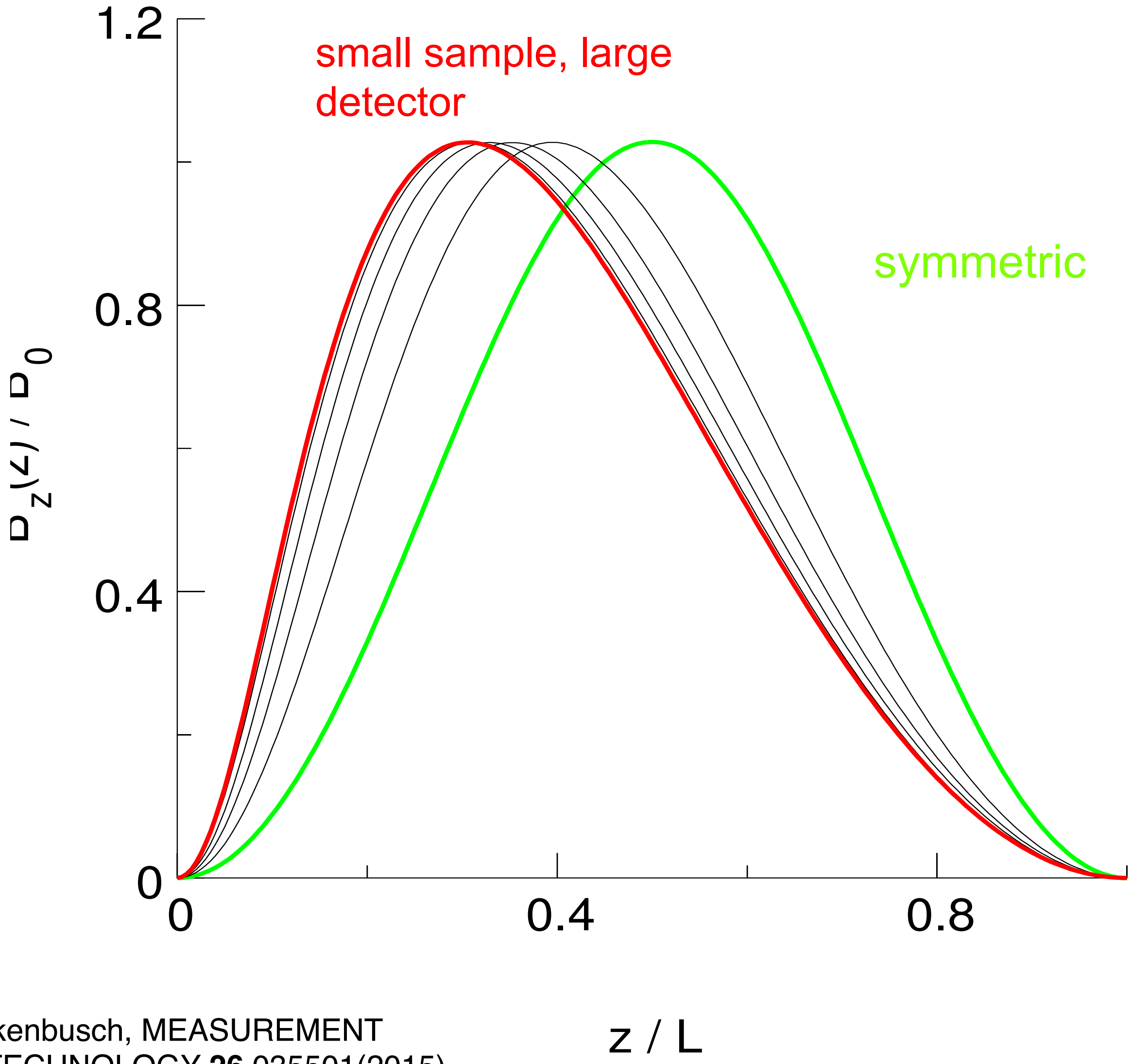
with

$$U = \int_{-L/2}^{L/2} z \beta(z) \mathrm{d}z, \qquad (16)$$

where $r^2(z) = (r_0 + z\tan\theta)^2$ and $\langle \cdots \rangle$ denotes the average over the path parameters r_0 and θ within the beam defining path ensemble.

Anzatz: $$B_z(z) = B_0 \; y(z)^2,$$ y = Fourier series

Field shape B(z)



S.Pasini, M.Monkenbusch, MEASUREMENT SCIENCE AND TECHNOLOGY **26** 035501(2015)

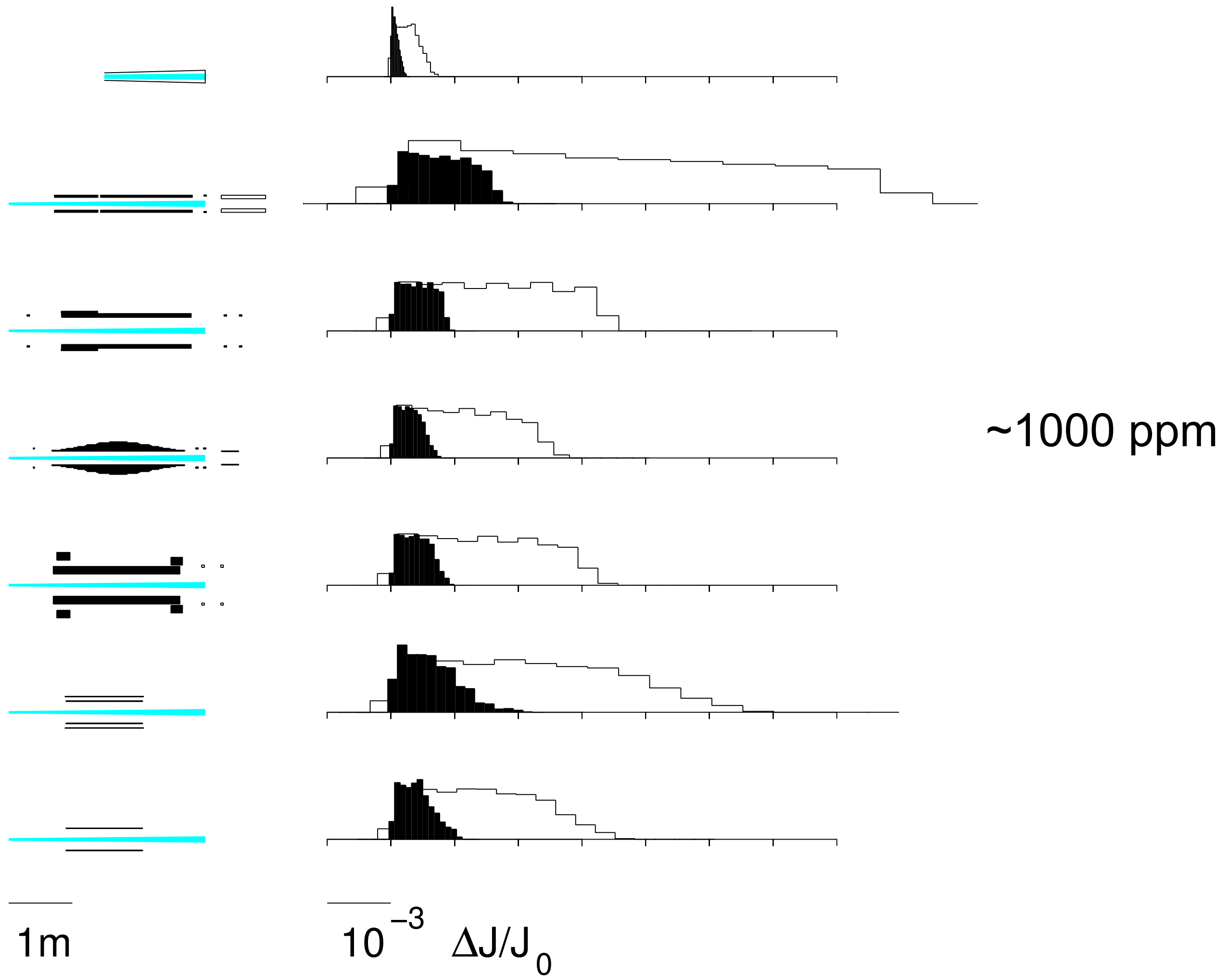
What is the lowest possible rms inhomogeneity ?

$$
\begin{aligned}
\langle \Delta J^2 \rangle = & \langle r_0^4 \rangle H^2 + \langle \tan^4 \theta \rangle G^2 + \langle (2r_0 \tan \theta)^2 \rangle U^2 + 2\langle r_0^2 \tan^2 \theta \rangle GH \\
& + 2\langle 2r_0 \tan^3 \theta \rangle GU + 2\langle 2r_0^3 \tan \theta \rangle HU,
\end{aligned}
$$

→ **215 ppm**

for 4cm sample, 20cm det (at pi/2)

The ‚older‘ instruments



Numerical optimisation..

$$\sum_{l=1}^{N} a_l^1 \, I_l = J_1 - \vec{B}_o \cdot \vec{L}_1$$

$$\sum_{l=1}^{N} a_l^2 \, I_l = J_2 - \vec{B}_o \cdot \vec{L}_2$$

$$\sum_{l=1}^{N} b_l^{i,j} \, I_l = B_j(\vec{x}_i) - B_{o,j}(\vec{x}_i)$$

$$\sum_{l=1}^{N} (c_l^c - \delta_{l,c}) \, I_l = I_{fixed}^c$$

...to have a functioning NSE spectrometer....

$$\Delta_{\text{inhom}} = \sqrt{\frac{1}{N_{\text{paths}}} \sum_{i=1}^{N_{\text{paths}}} (J_i - \langle J \rangle)^2}$$

$$\Delta_{\text{loc}} = \sqrt{\sum_{i=1}^{N_{\text{loc}}} |\vec{B}(\vec{x}_i) - \vec{B}_i^{\text{aimed}}|^2}$$

$$\Delta_{\text{depol}} = \frac{v}{2\pi\gamma} \sum_{i=1}^{N_{\text{depol}}} \left| \frac{\delta B_\perp(\vec{x}_i)}{\vec{x}_i - \vec{x}_{i+1}} \right| \frac{1}{B(\vec{x}_i)^2}$$

$$\Delta_{\text{fringe}} = \sum_{i=1}^{N_{\text{fringe}}} |\vec{B}^{\text{mainset1}}(\vec{x}_i^{\text{fringe}})|$$

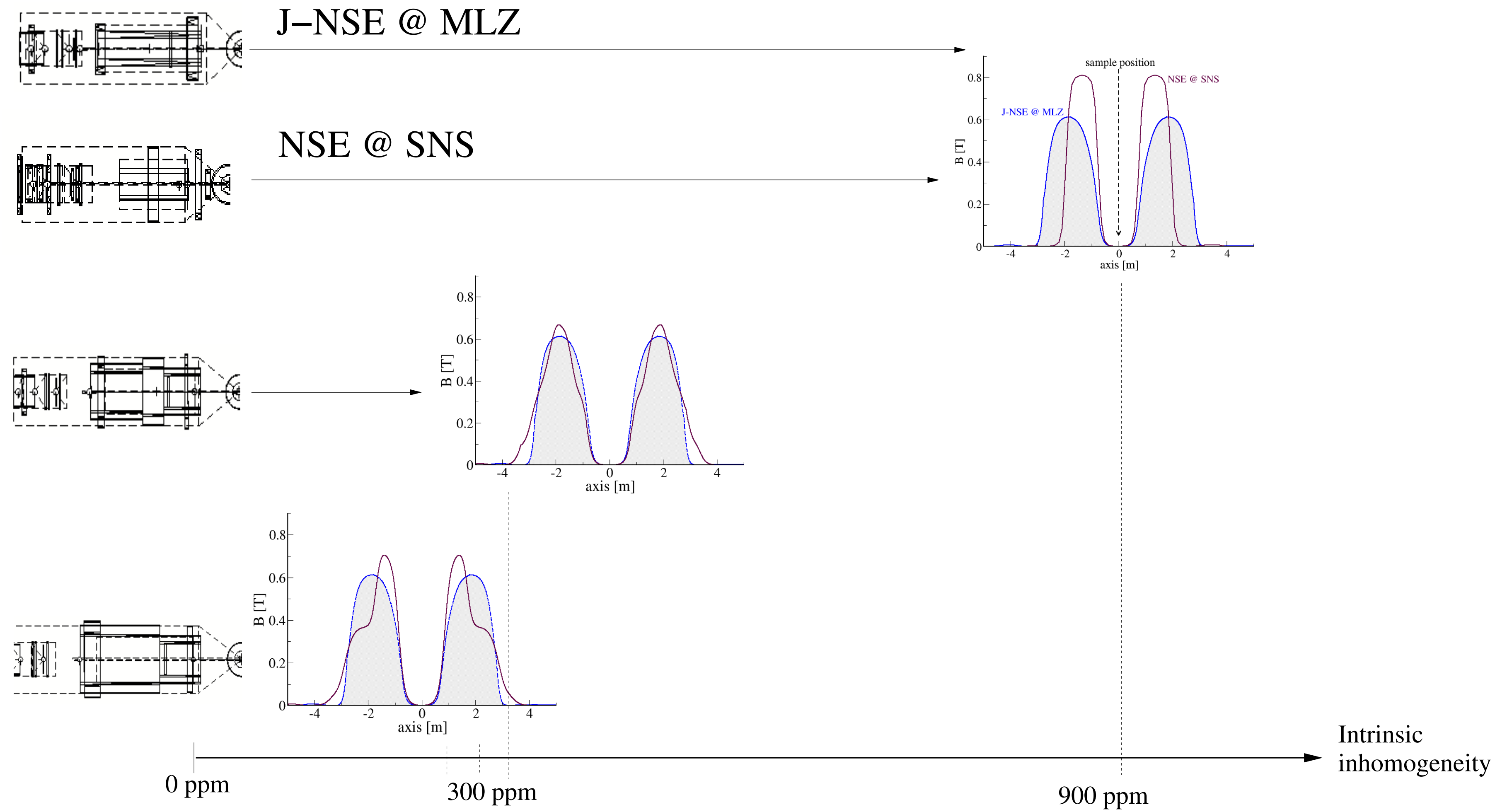
..to reduce inhomogeneity ..

$$\Delta_{\text{ccx}} = |I_{\text{ccx}}|.$$

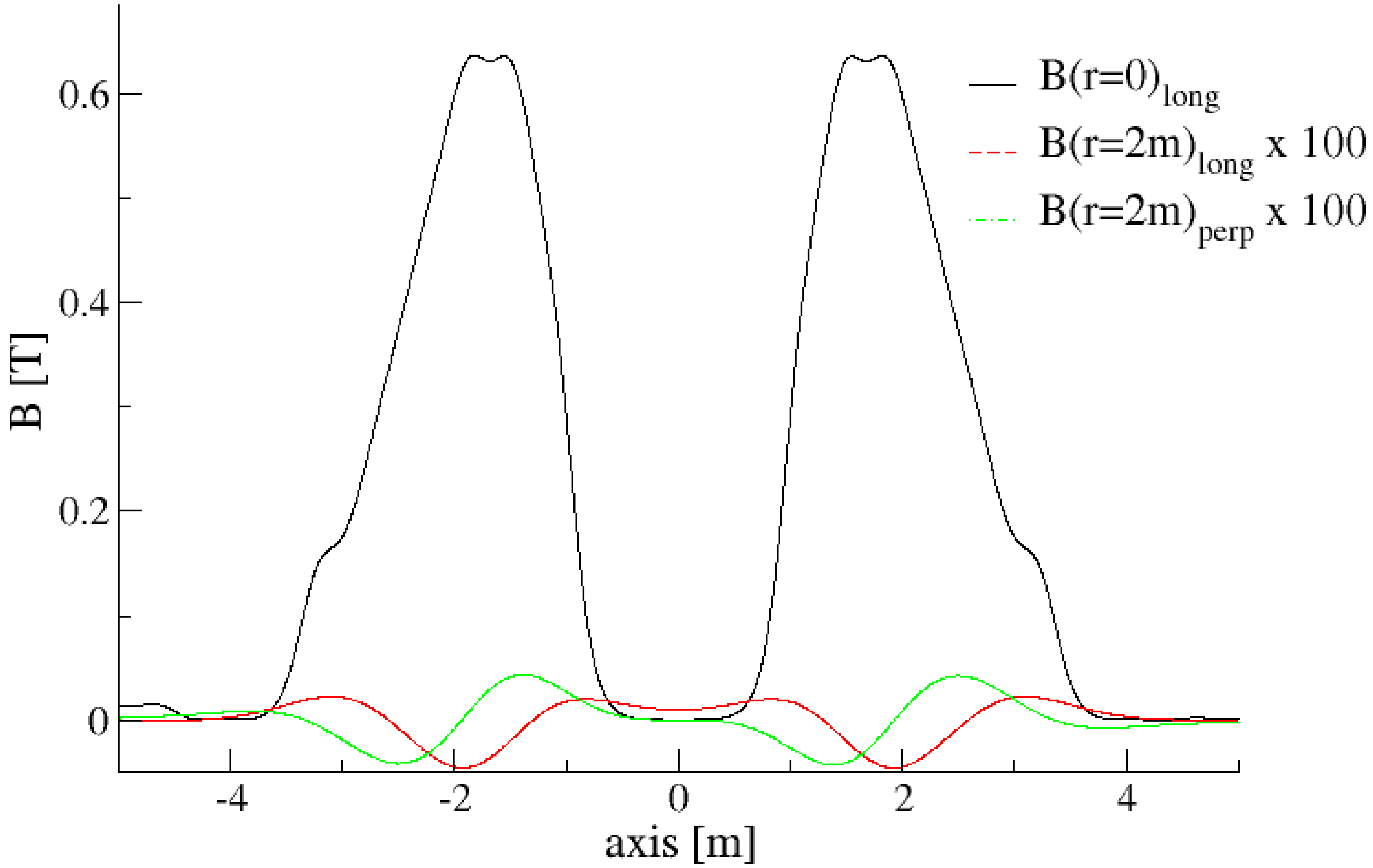
$$\Delta_{\text{hpi}} = s|\vec{B}(\vec{x}_{\pi/2}) - \vec{B}(\vec{x}_{\pi/2} + \hat{e}_z \, d)|^2$$

minimize

$$\Delta = \sum_{X=1}^{7} W_x \Delta_X$$

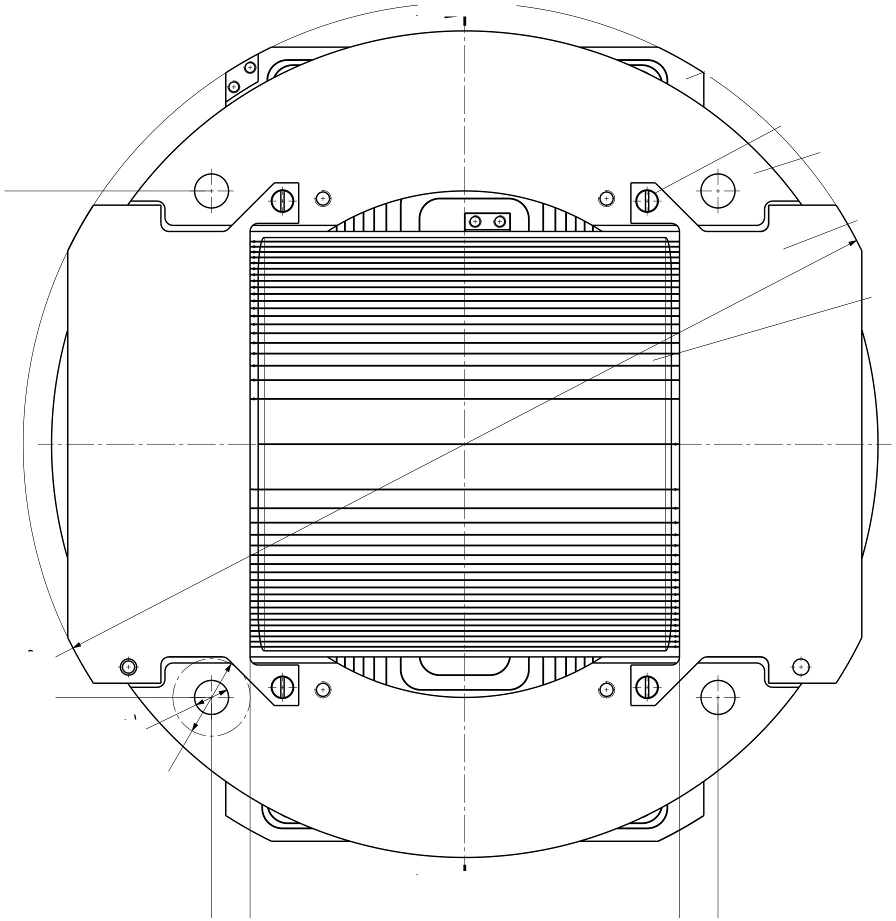

J–NSE @ MLZ
NSE @ SNS
sample position
NSE @ SNS
J-NSE @ MLZ
B [T]
axis [m]
Intrinsic inhomogeneity
0 ppm
300 ppm
900 ppm

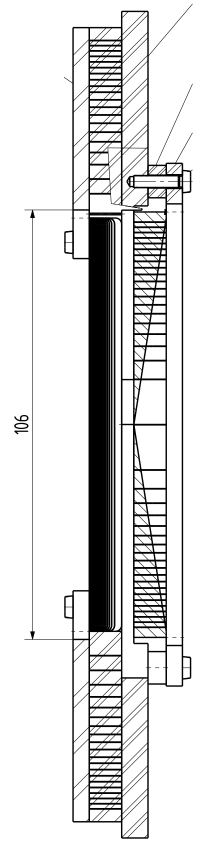
B(z)

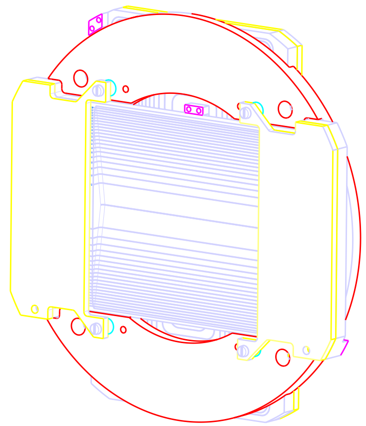


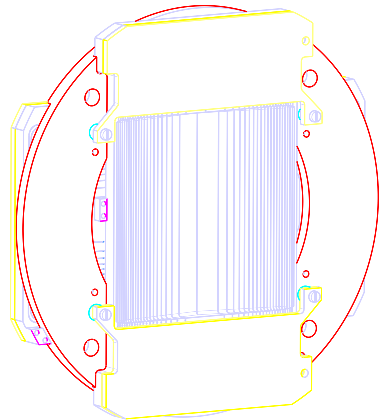
B(r=0)long
B(r=2m)long x 100
B(r=2m)perp x 100
B [T]
0.6
0.4
0.2
0
-4
-2
0
2
4
axis [m]

Correction element









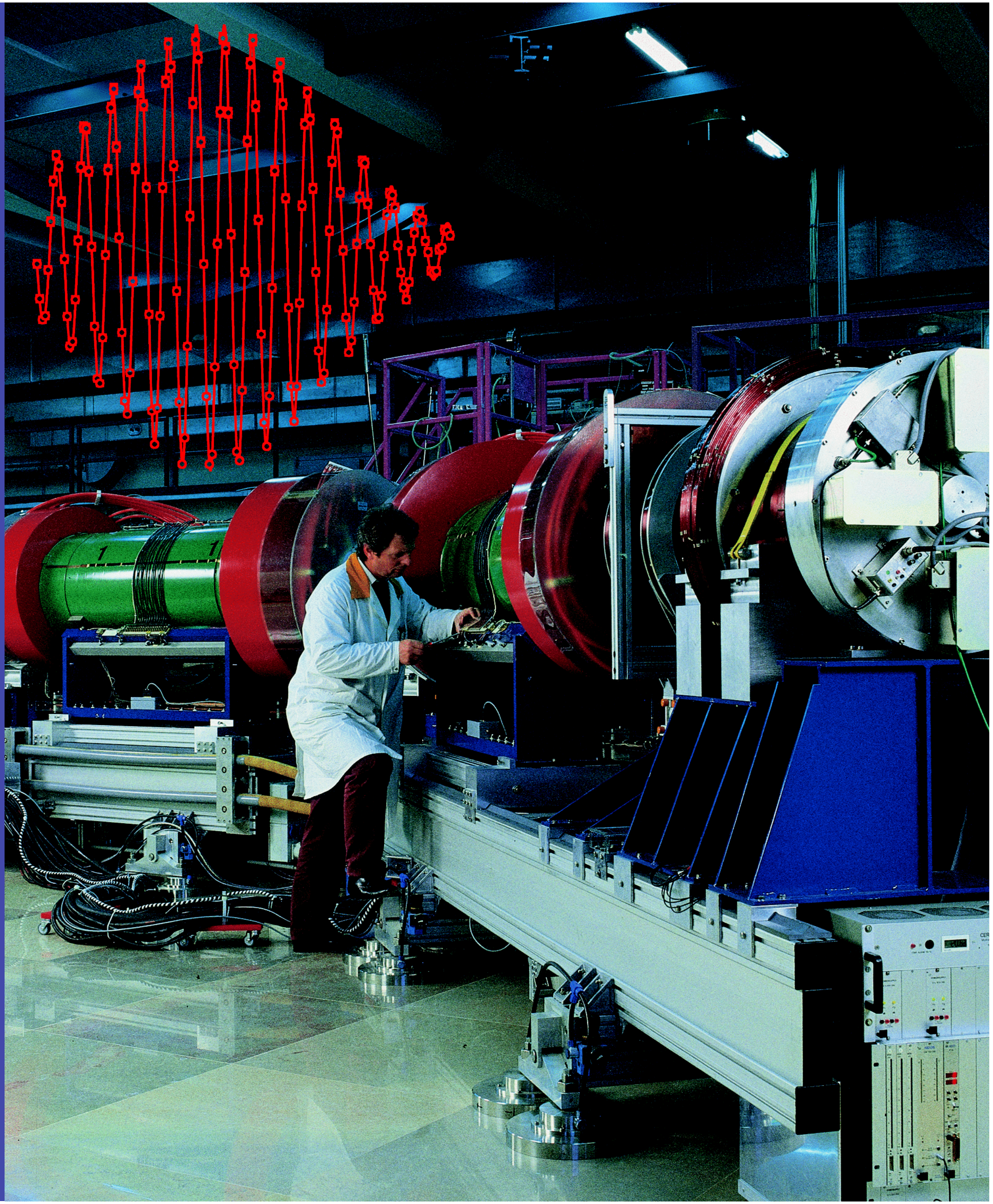
FRJ2-NSE

1996

ELLA

→now →

@ FRM II



Apr 2018

J-NSE

2006-2017

"old"

J-NSE

2006-2017

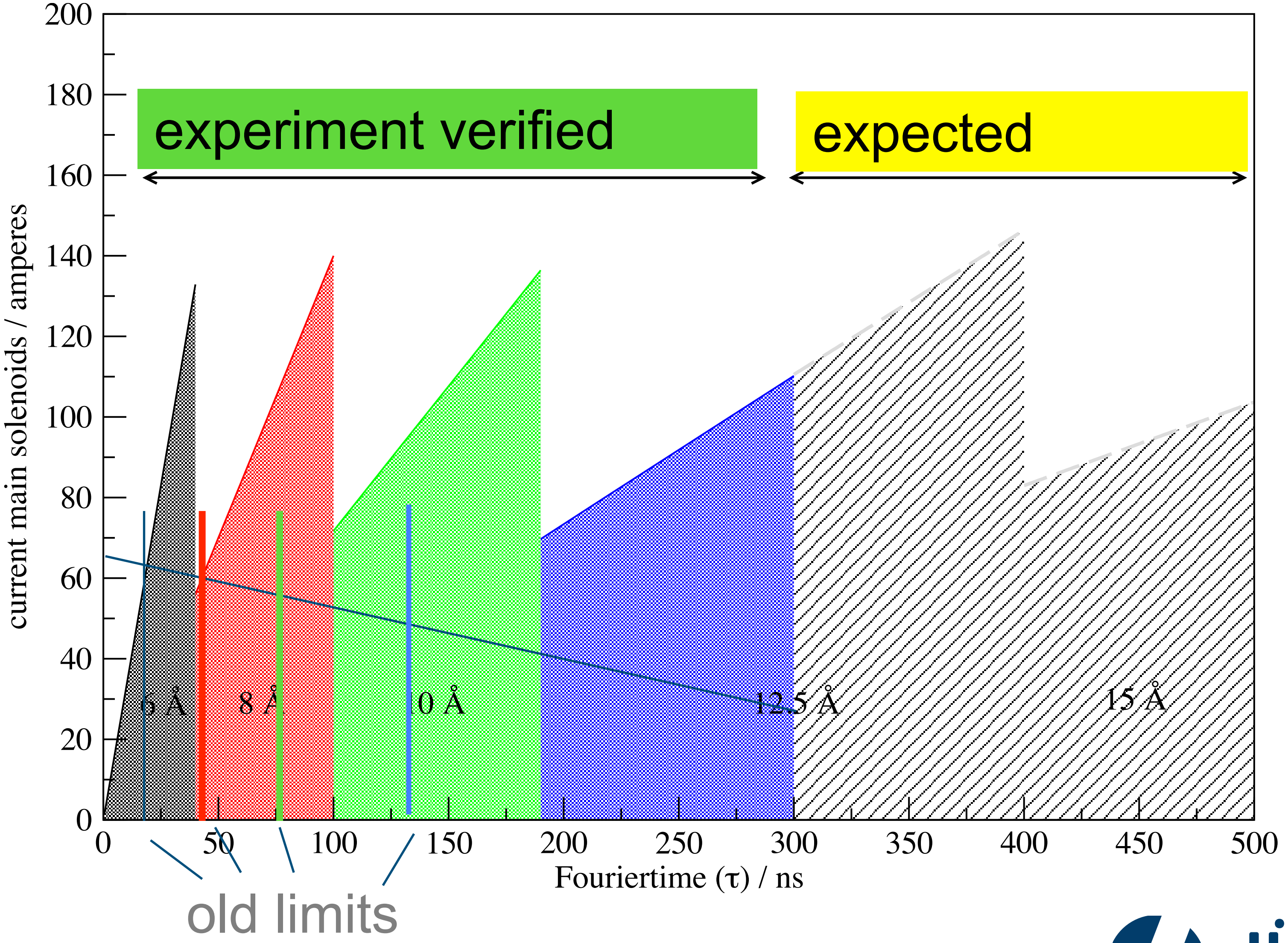
Apr 2018

J-NSE "PHOENIX"

Apr 2018

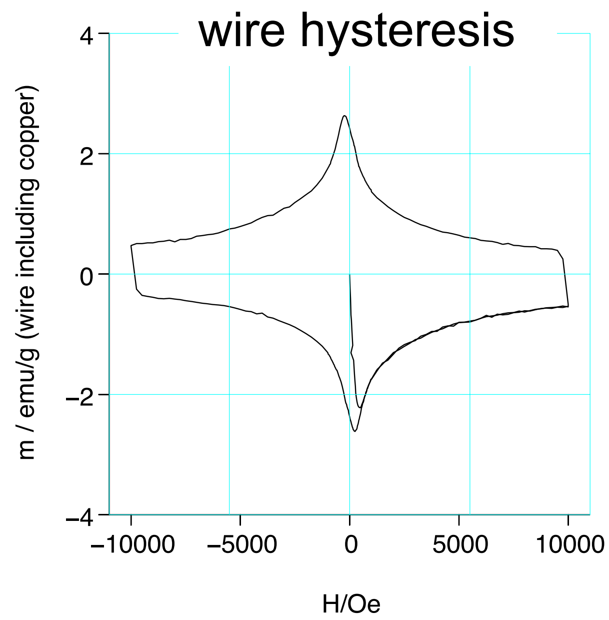
JÜLICH
Forschungszentrum

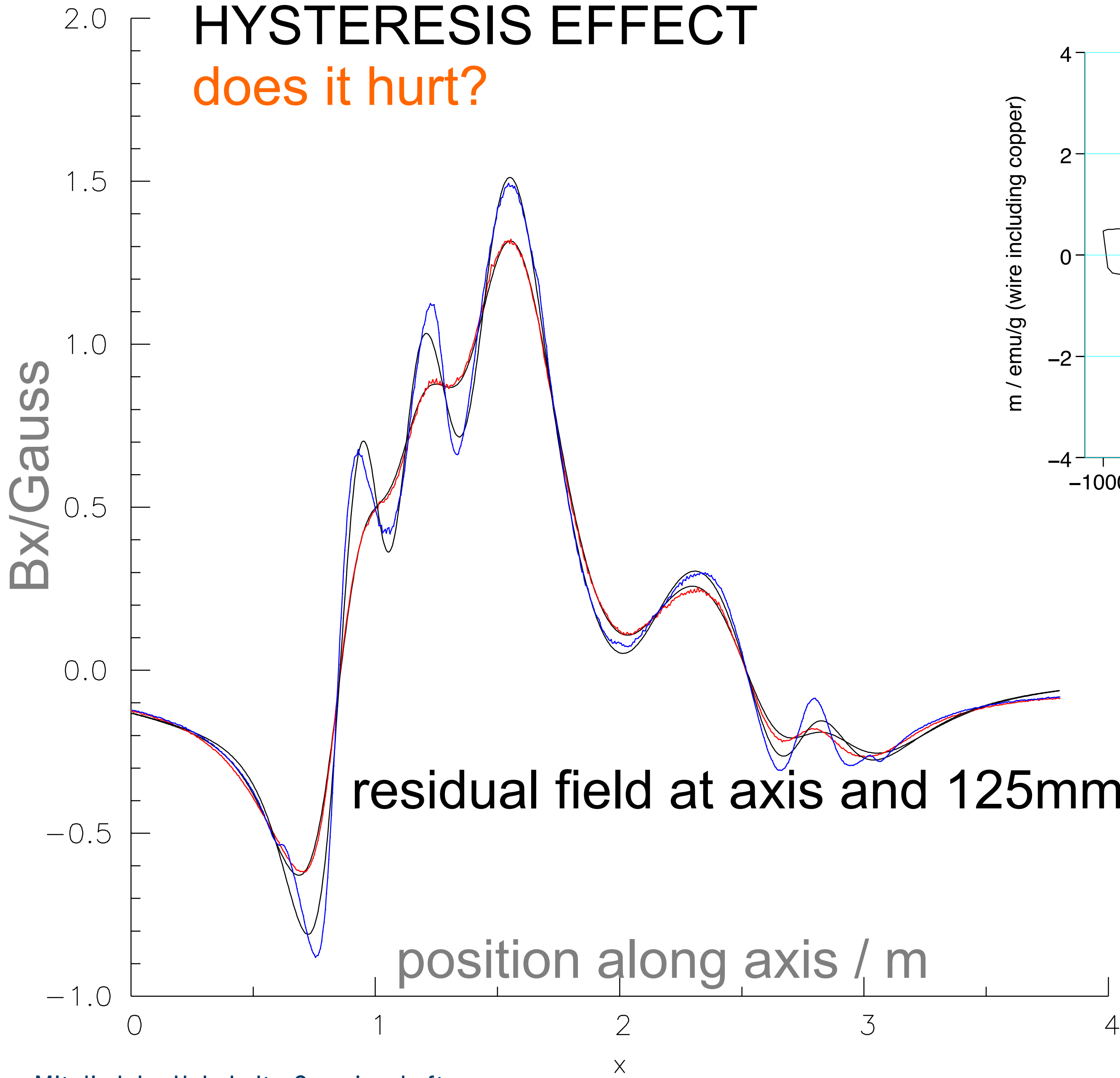
J-NSE new ranges



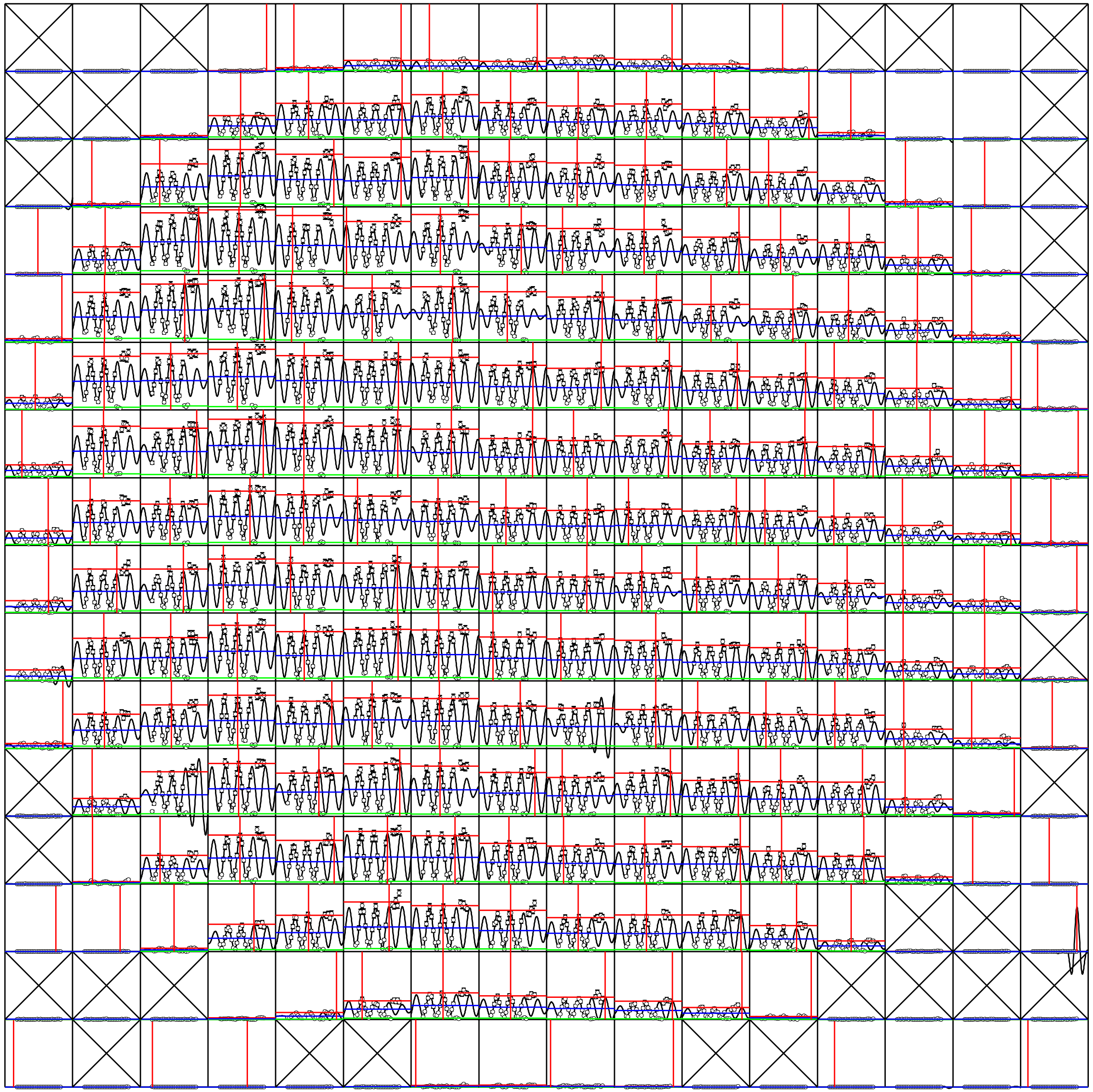
HYSTERESIS EFFECT

does it hurt?





residual field at axis and 125mm off axis

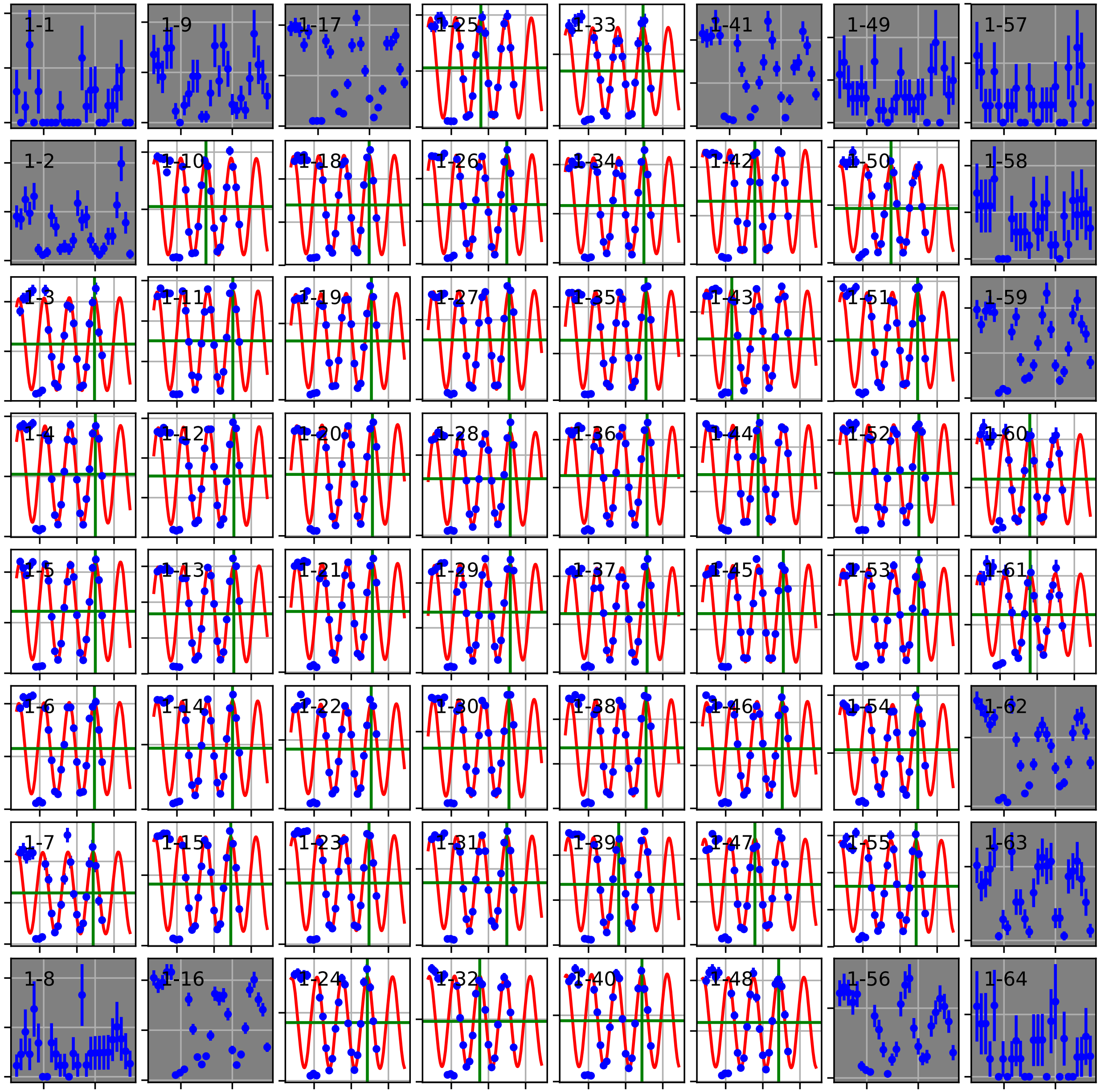


1 ns
8 A
ref

Apr 2018

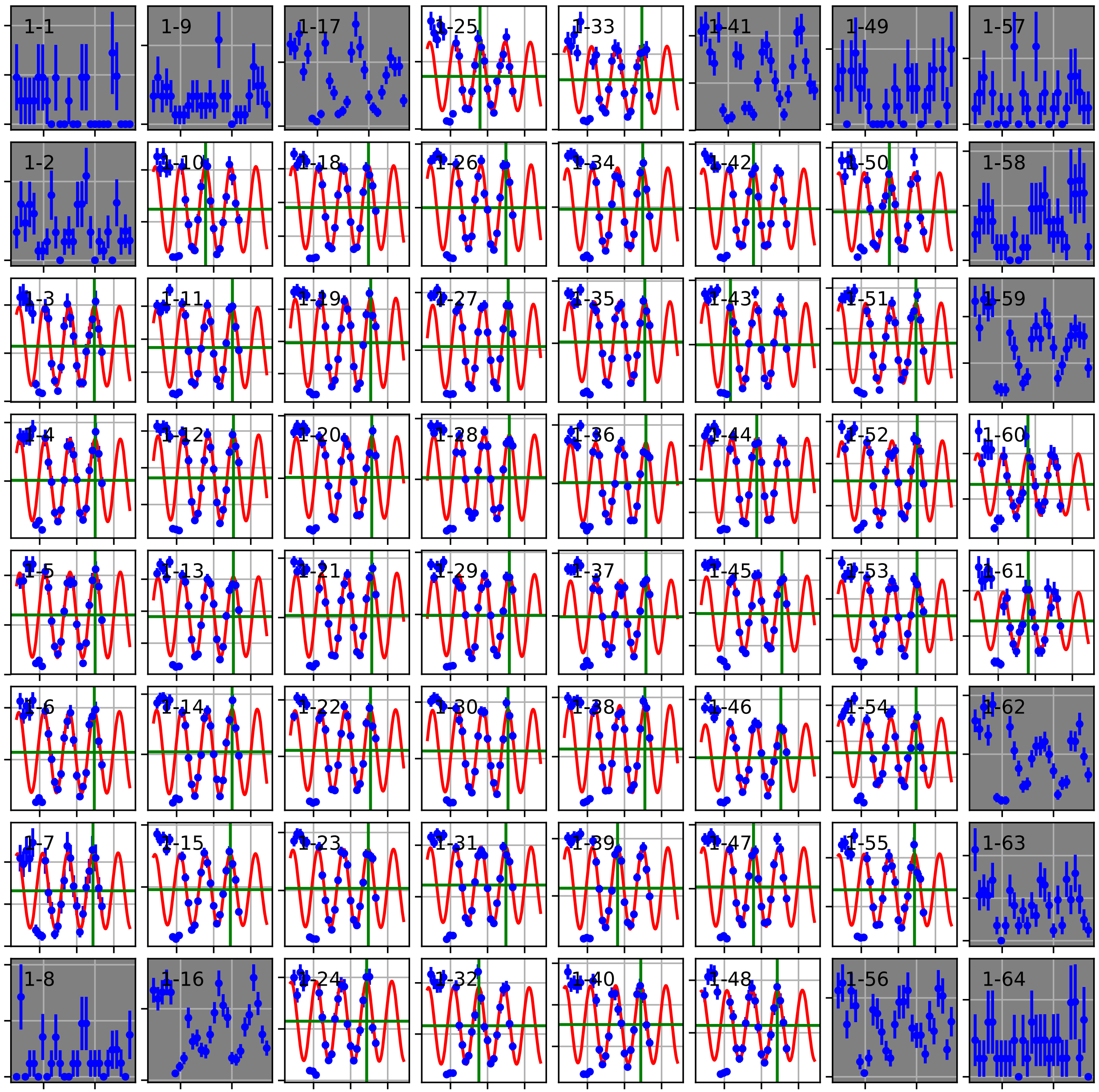
ActC4mm (./fits_200421 echo[1])

ref 1ns (8A): full echo in all pixels: **NO** bad hysteresis effects



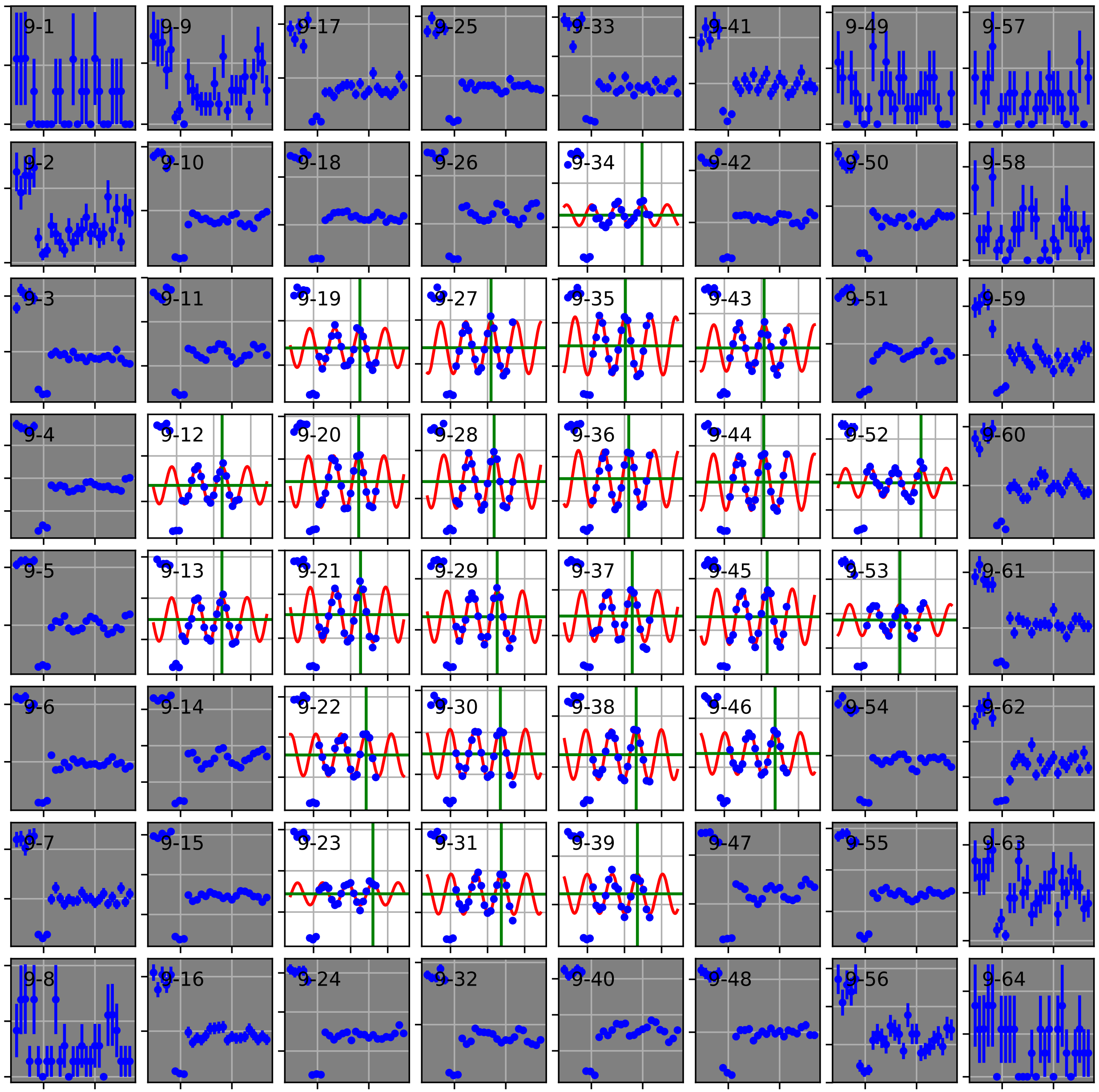
PI80klin (./fits_200481 echo[1])

Polymer melt 1ns (8A): only slight reduction of echo amplitude



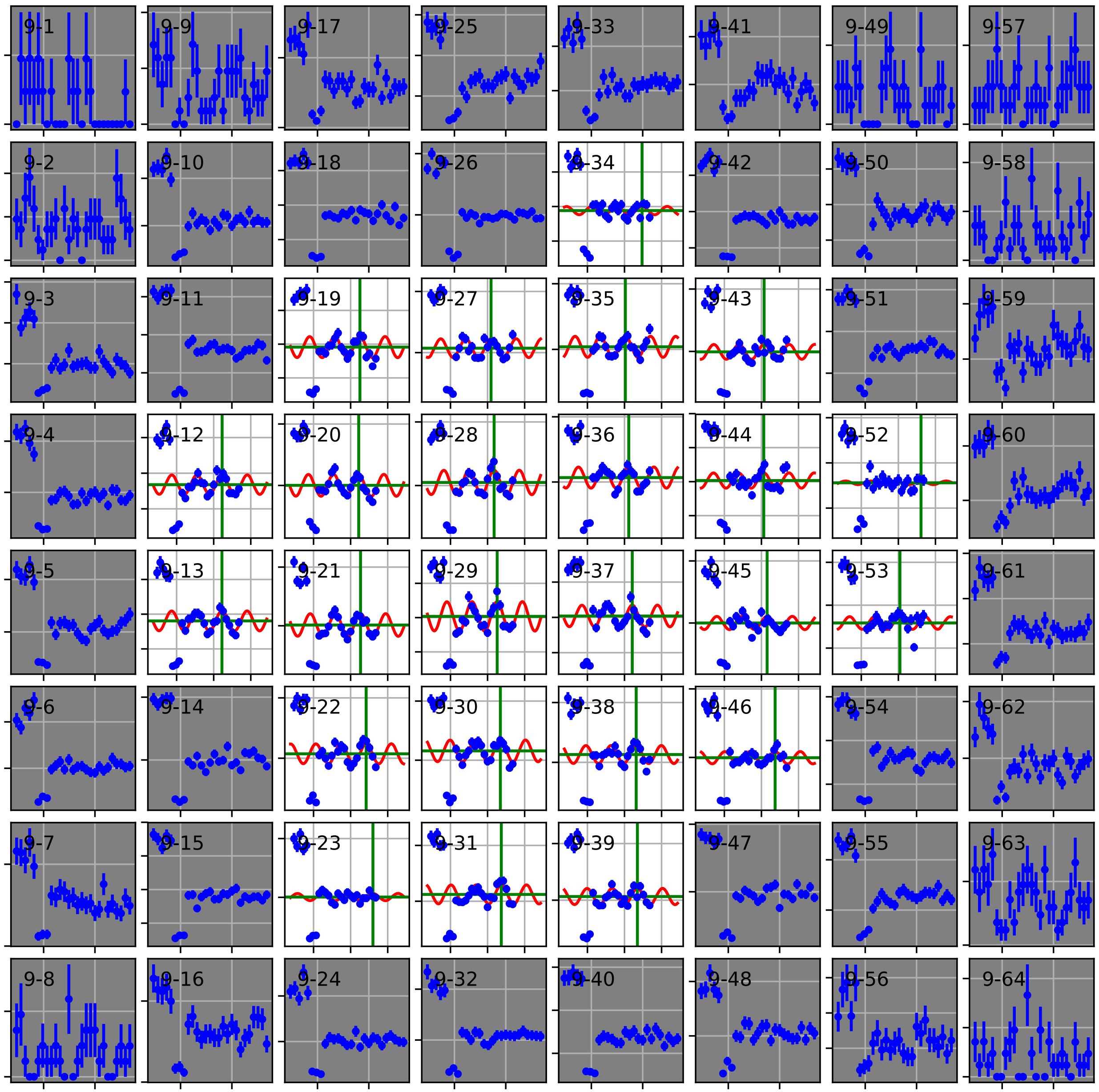
ActC4mm (./fits_200421 echo[9])

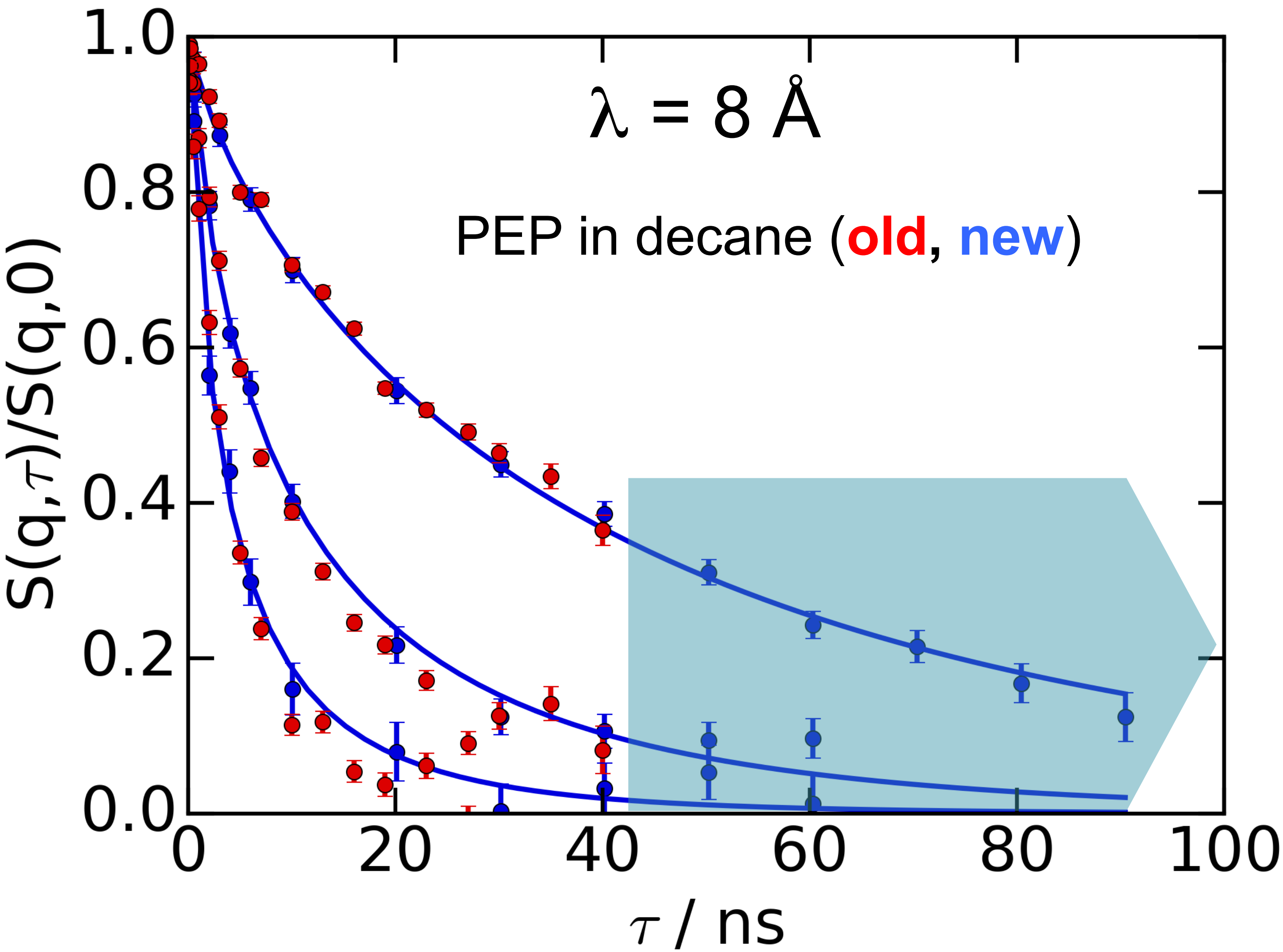
ref 90ns (8A): good echos in central field (correction effective)



PI80klin (./fits_200481 echo[9])

Polymer 90ns (8A): reduced echoes (relaxation compared to ref)




λ = 8 Å
PEP in decane (old, new)
S(q,τ)/S(q,0)
τ / ns
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100

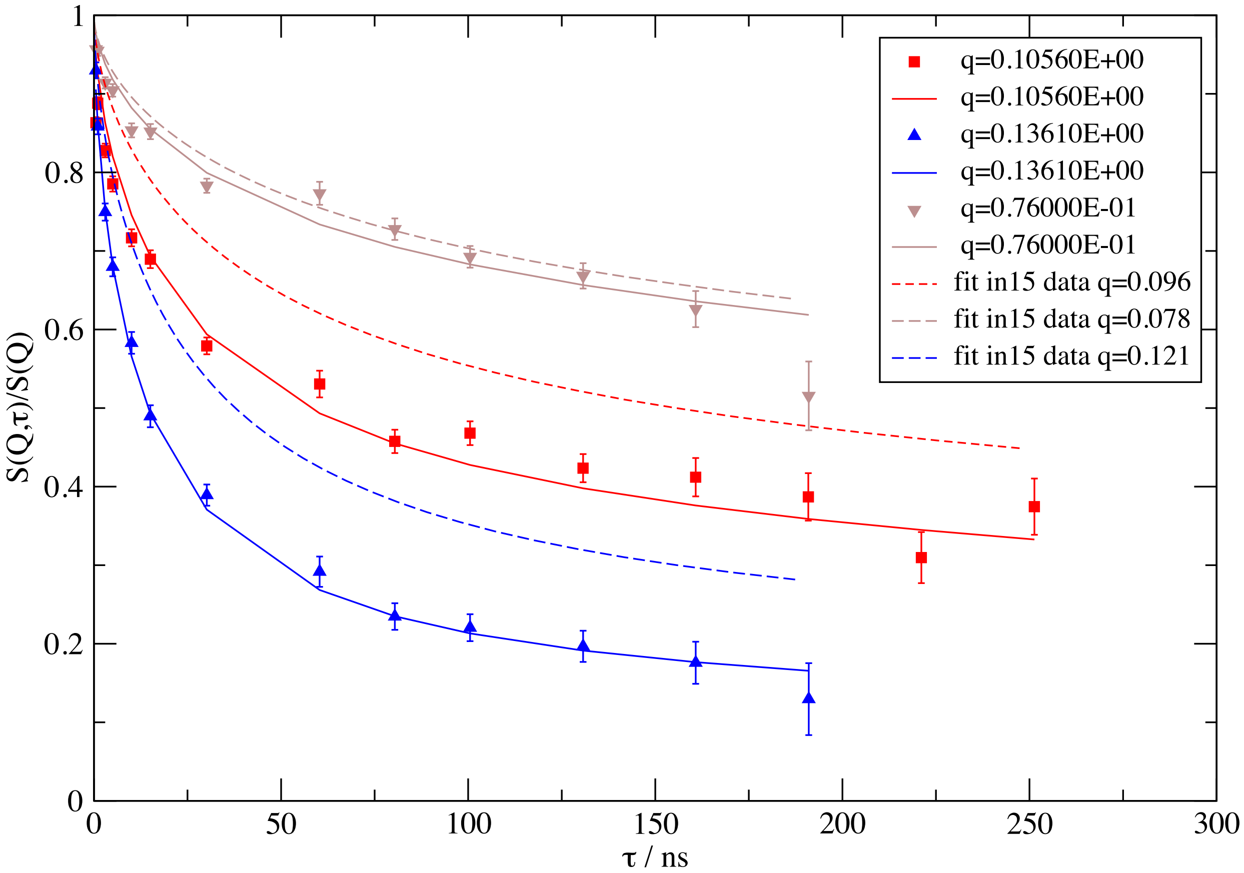


Figure 2: JNSE vs. IN15. The dashed lines are the fitted theory for the IN15 old data (as a global fit); they are re-computed with tau and Wl⁴ (see theory in the text) rescaled by a factor 1.4, solid curves. The re-computed curves can be compared with the JNSE data (symbols). The solid curves are not a fit of the JNSE data. For sake of clarity the old IN15 data are not shown.

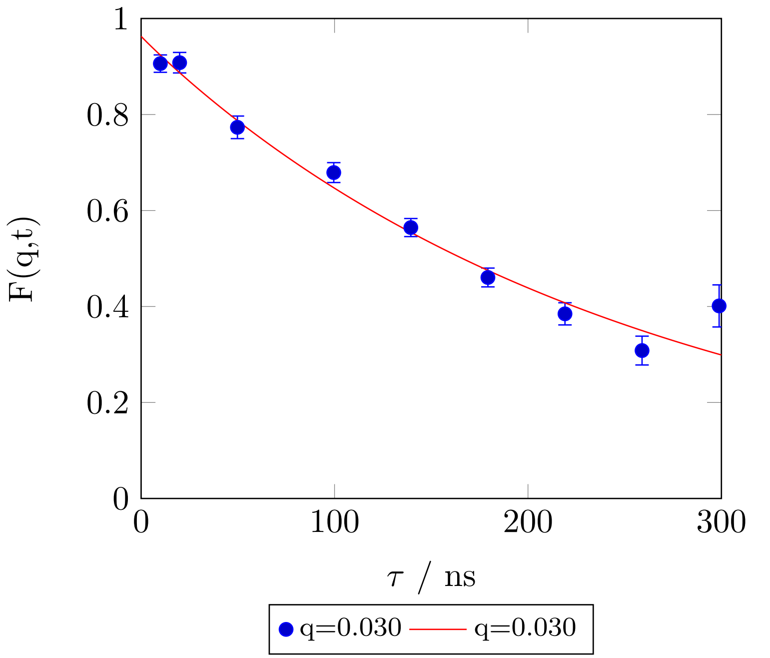
A “real world example”:

protein solution (3% in D2O)

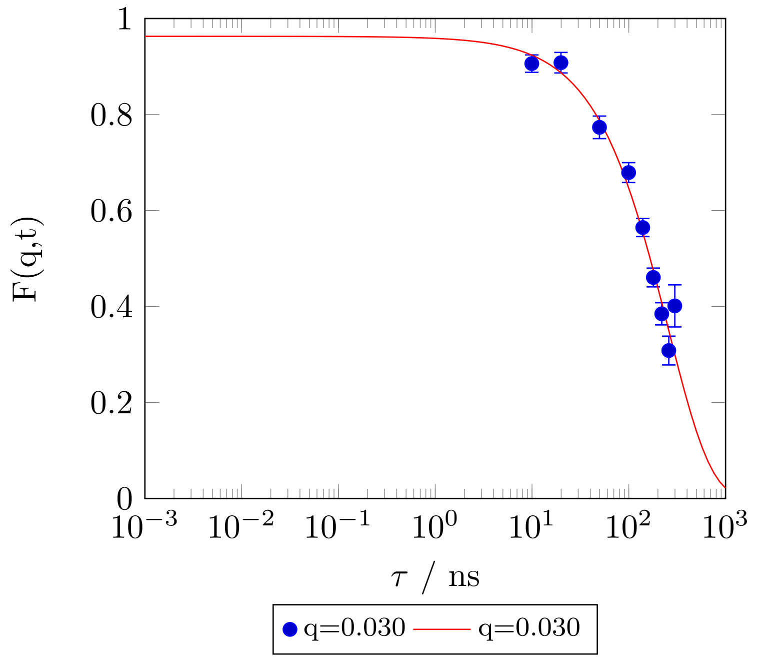
using different wavelengths from 6 to 12.5 Å

and ***DrSpine*** (under development) for evaluation

apoMbpD6_"apoMb_pD6_3_percent_ [1, 800]
With background subtraction: transmission factor= 1.0000 **volfrac=** 1.0000



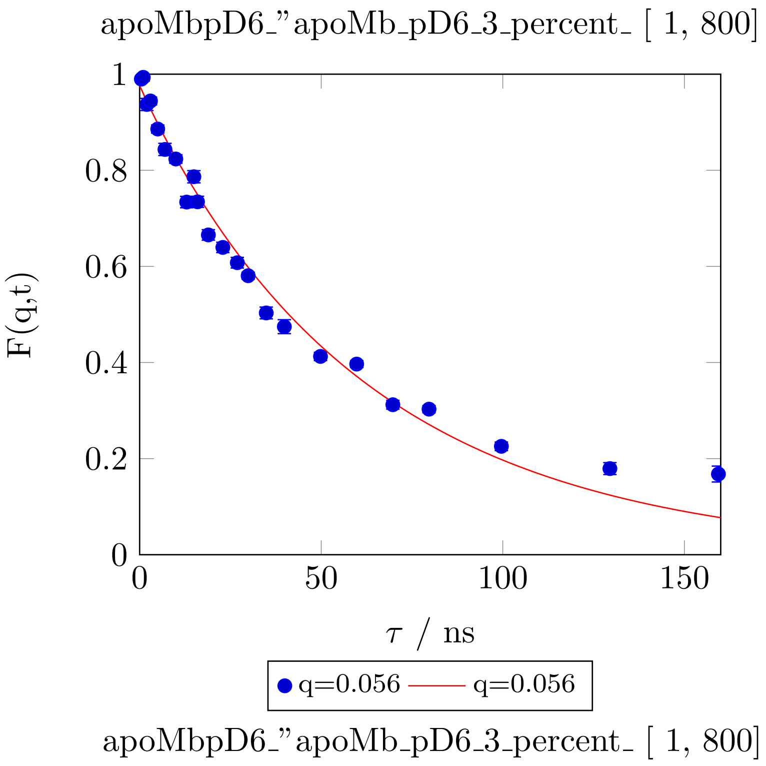
apoMbpD6_"apoMb_pD6_3_percent_ [1, 800]

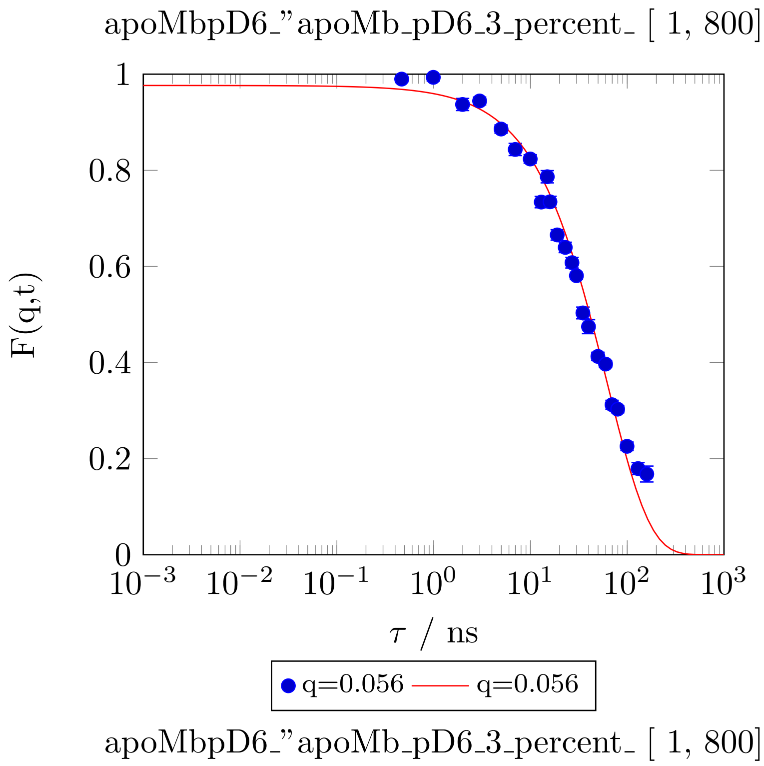


apoMbpD6_"apoMb_pD6_3_percent_ [1, 800]

λ = 12.5Å

apoMbpD6_"apoMb_pD6_3_percent_ [1, 800]
With background subtraction: transmission factor= 1.0000 **volfrac=** 1.0000

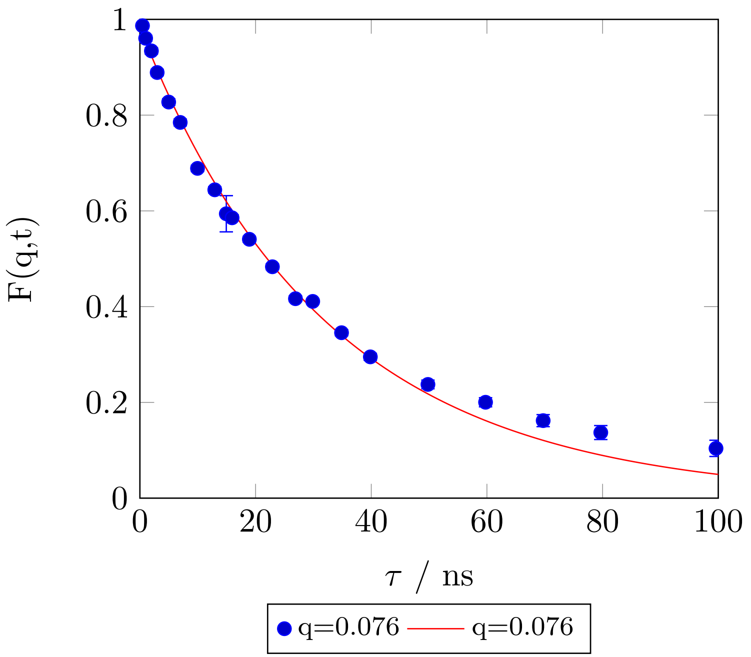




λ = 10Å

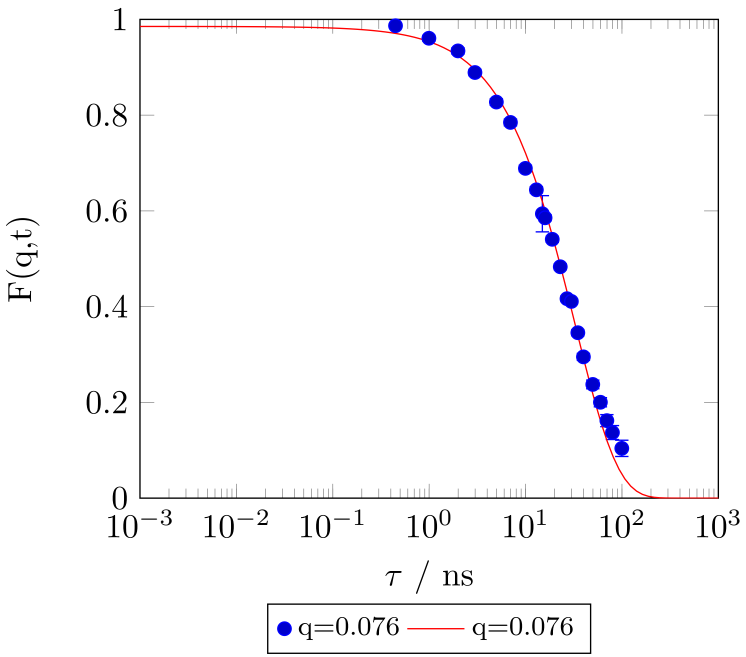
apoMbpD6_"apoMb_pD6_3_percent_ [1, 800]
With background subtraction: transmission factor= 1.0000 **volfrac=** 1.0000

apoMbpD6_"apoMb_pD6_3_percent_ [1, 800]



apoMbpD6_"apoMb_pD6_3_percent_ [1, 800]

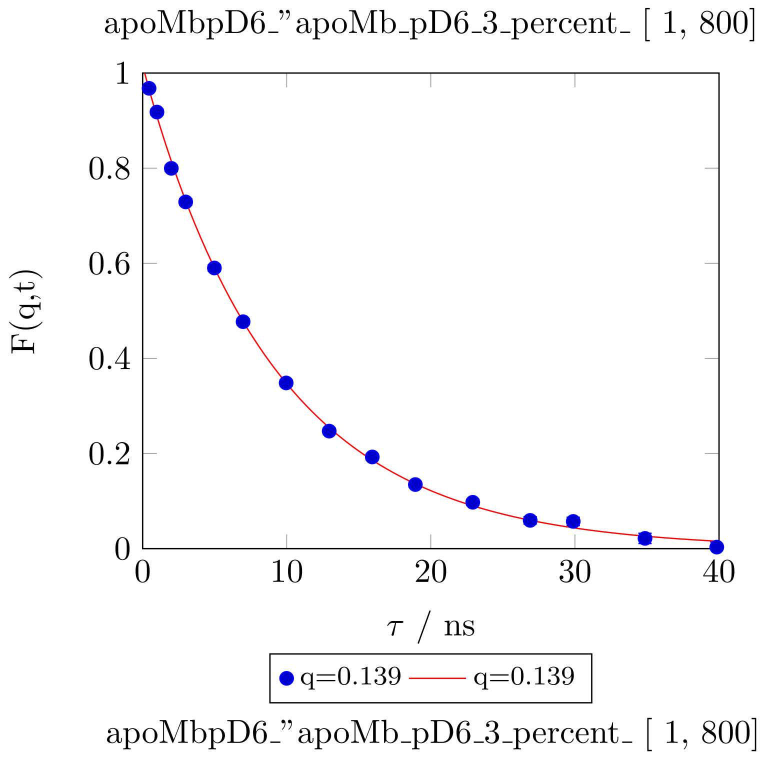
apoMbpD6_"apoMb_pD6_3_percent_ [1, 800]

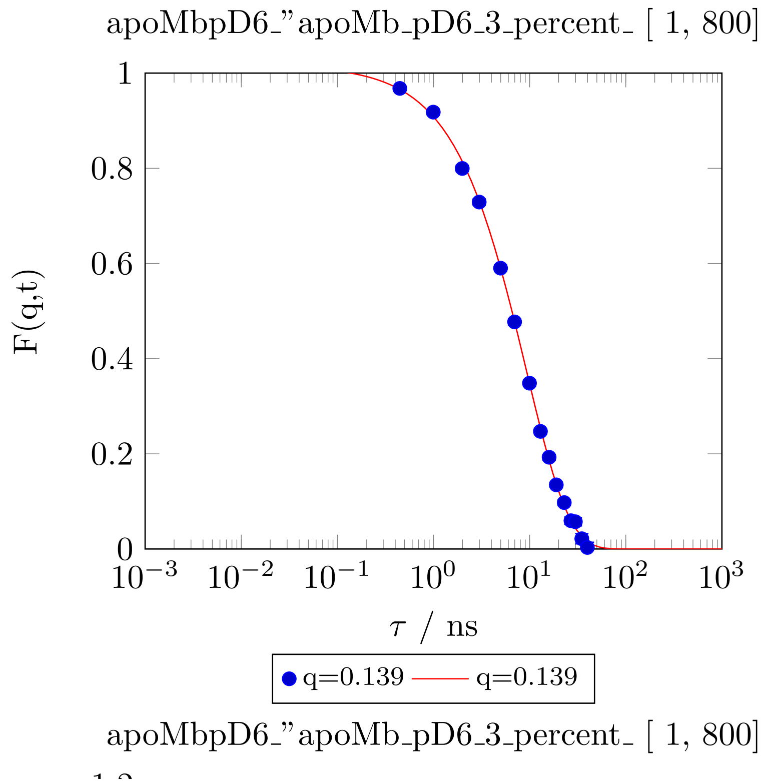


apoMbpD6_"apoMb_pD6_3_percent_ [1, 800]

λ = 8Å

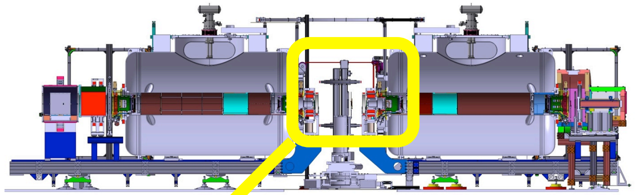
apoMbpD6_"apoMb_pD6_3_percent_ [1, 800]
With background subtraction: transmission factor= 1.0000 **volfrac=** 1.0000

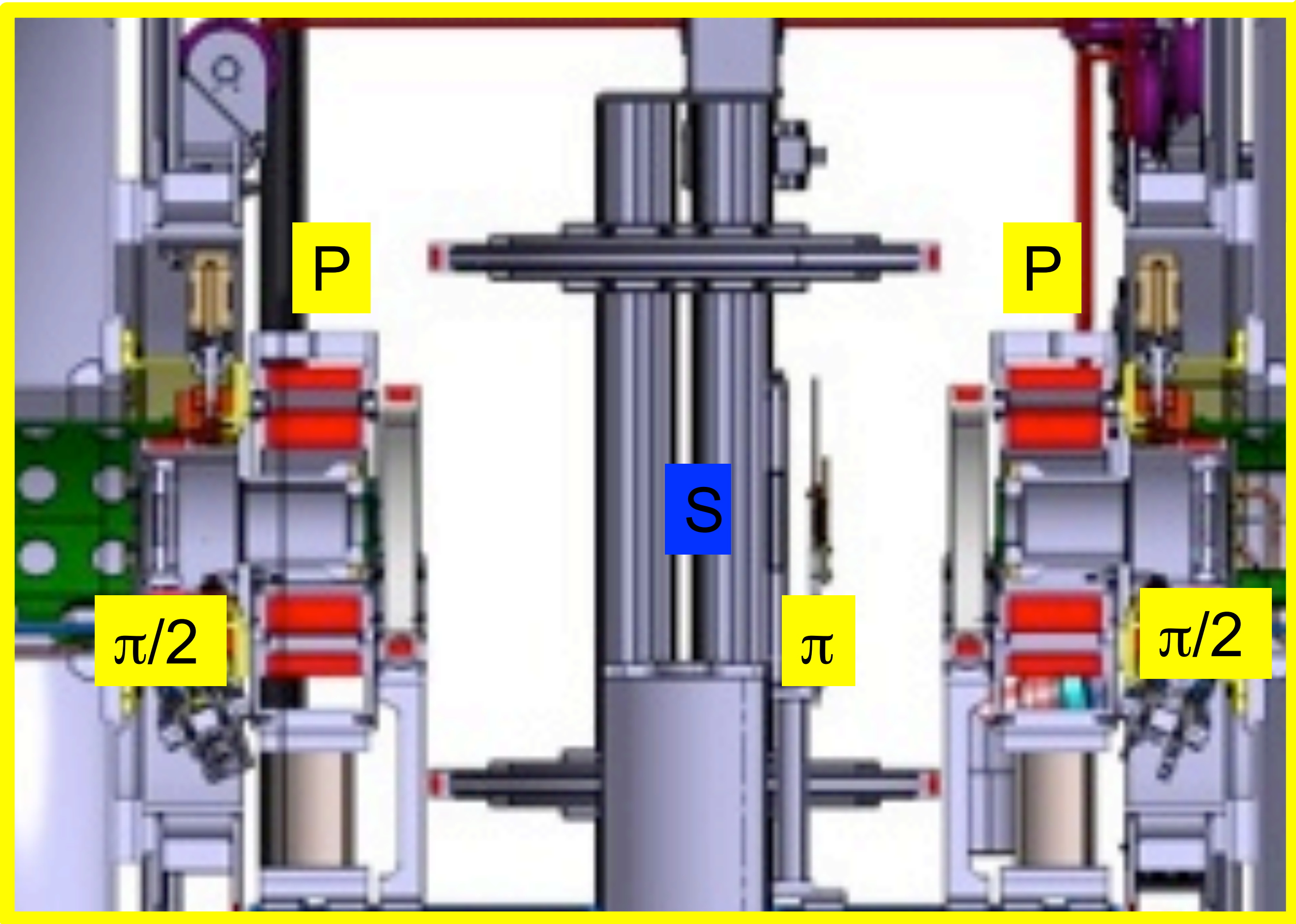




λ = 6Å

Extension to short times
"Shorty"





P = precession

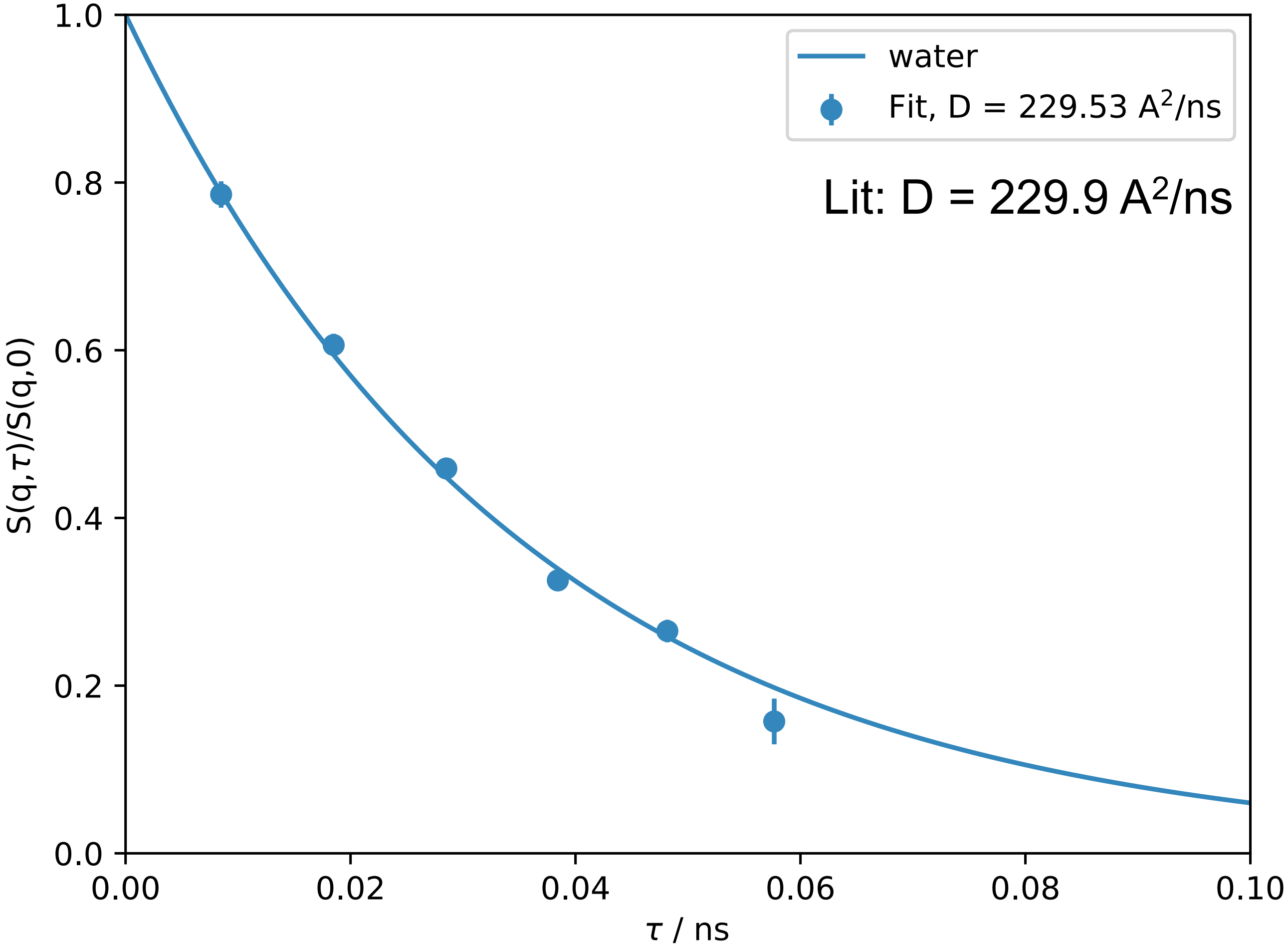
π/2 : flipper

π : flipper

S : sample

“Shorty” demo experiment: incoherent scattering from H2O

Q=0.35 Å^{-1}



Thank you for your attention !